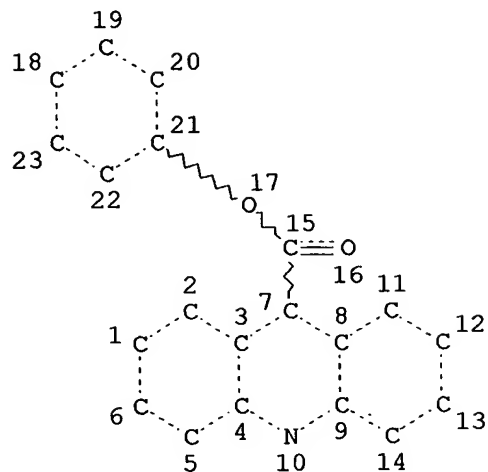


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L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

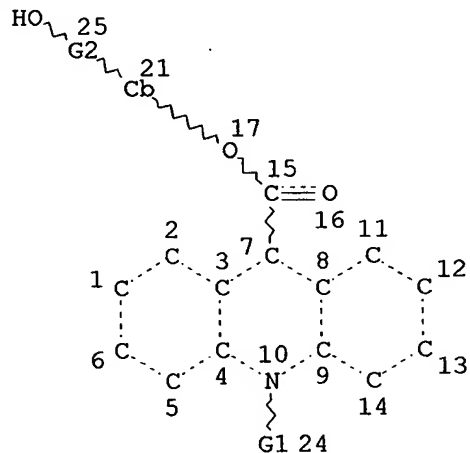
NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L2 797 SEA FILE=REGISTRY SSS FUL L1

L3 STR

26



VAR G1=H/A

REP G2=(0-20) A

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 21

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E6 C AT 21

GRAPH ATTRIBUTES:

RSPEC 7

NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L4 174 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
L6 7820 SEA FILE=HCAPLUS ABB=ON PLU=ON "LUMINESCENCE, CHEMILUMINESCEN
CE"+OLD,NT/CT
L7 2475 SEA FILE=HCAPLUS ABB=ON PLU=ON CHEMILUMINESCENCE SPECTROSCOPY
+OLD,NT/CT
L8 704 SEA FILE=HCAPLUS ABB=ON PLU=ON CHEMILUMINESCENT SUBSTANCES+OL
D/CT
L10 31 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND ((L6 OR L7 OR L8) OR
CHEMILUM?)

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L10 ANSWER 1 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:20978 HCAPLUS

DOCUMENT NUMBER: 138:86124

TITLE: Acridinium ester labels having hydrophilic modifiers

INVENTOR(S): Natrajan, Anand; Sharpe, David; Jiang, Qingping

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: Eur. Pat. Appl., 28 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| EP 1273917 | A2 | 20030108 | EP 2002-13902 | 20020621 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| US 2003045716 | A1 | 20030306 | US 2001-898381 | 20010703 |
| JP 2003050204 | A2 | 20030221 | JP 2002-185836 | 20020626 |

PRIORITY APPLN. INFO.: US 2001-898381 A 20010703

AB The present invention is generally directed to detectable
chemiluminescent acridinium ester labels having hydrophilic
modifiers; to compns., complexes and/or conjugates which include such
labels; and to processes for performing bioanal. assays for target
analytes which use such labels. Assays for folate, theophylline, and
tobramycin (using such labels with hydrophilic modifiers such as nonionic
polyethylene glycol and polyionic spermine disulfonate and polyionic
spermine dicarboxylate) are described in detail.

IT **482648-38-4P**

RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic
preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant
or reagent); USES (Uses)

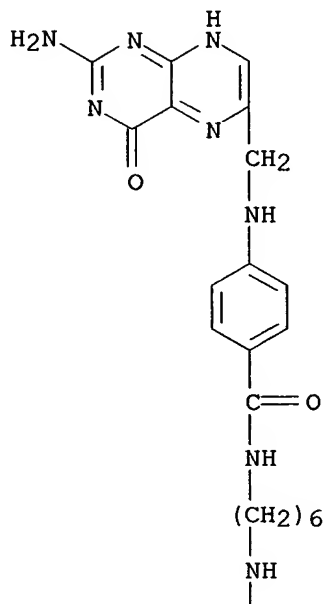
(NSP-DMAE-HD-PTEROATE; acridinium ester labels having hydrophilic
modifiers)

RN 482648-38-4 HCAPLUS

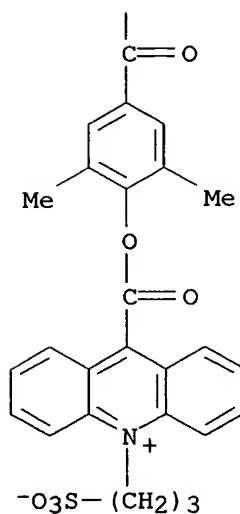
CN Acridinium, 9-[[4-[[[6-[[4-[[[2-amino-1,4-dihydro-4-oxo-6-

pteridiny]methyl]amino]benzoyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



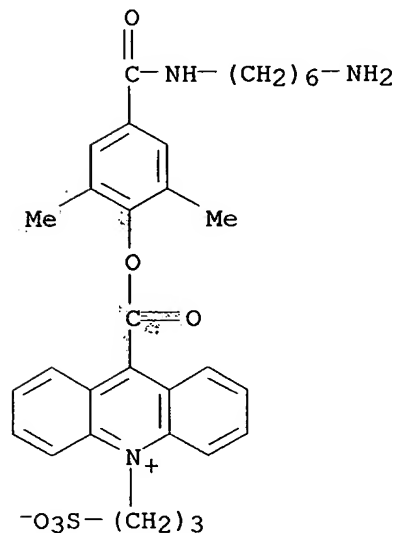
IT 194357-76-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(NSP-DMAE-HD; acridinium ester labels having hydrophilic modifiers)

RN 194357-76-1 HCAPLUS

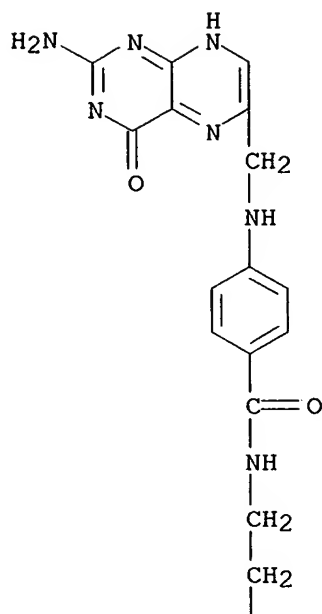
CN Acridinium, 9-[[4-[[[(6-aminohexyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

IT **482648-41-9P**RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(acridinium ester labels having hydrophilic modifiers)

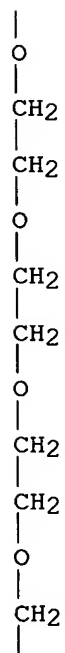
RN 482648-41-9 HCAPLUS

CN Acridinium, 9-[[4-[21-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]phenyl]-1,21-dioxo-5,8,11,14,17-pentaoxa-2,20-diazaheneicos-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

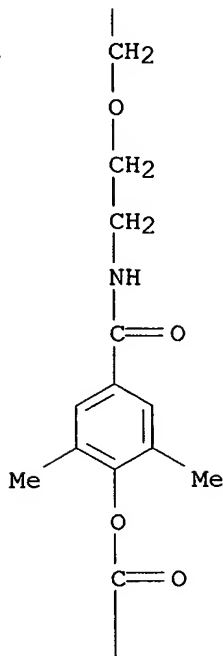
PAGE 1-A



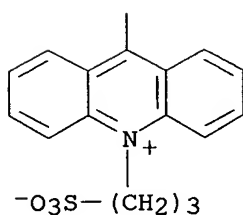
PAGE 2-A



PAGE 3-A



PAGE 4-A



IT 482648-46-4P 482648-48-6P 482648-49-7P
 482648-50-0P 482648-51-1P 482648-52-2P
 482648-53-3P 482648-54-4P 482648-56-6P
 482648-57-7P

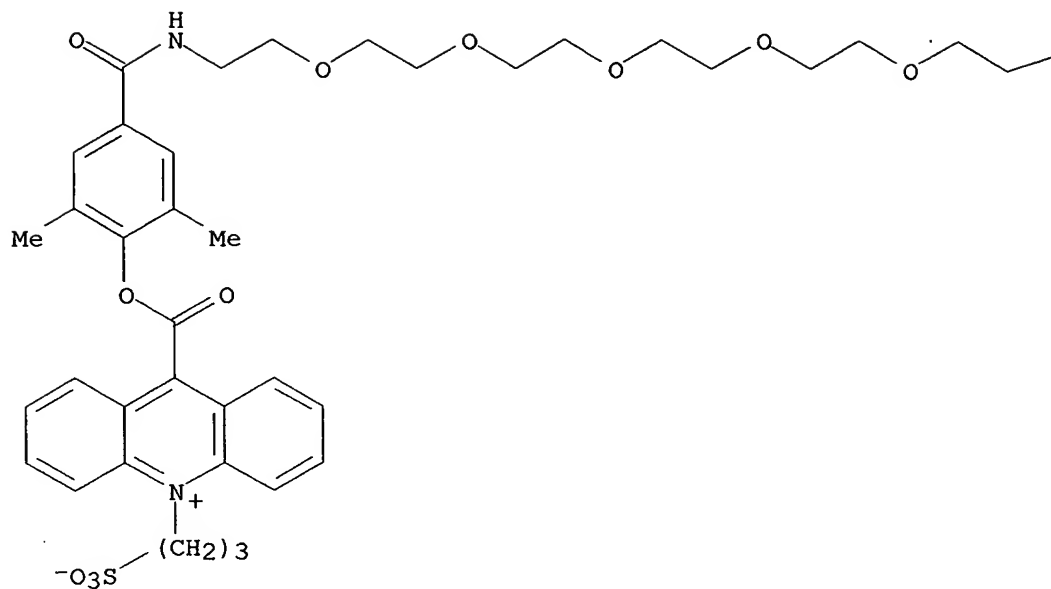
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (acridinium ester labels having hydrophilic modifiers)

RN 482648-46-4 HCAPLUS

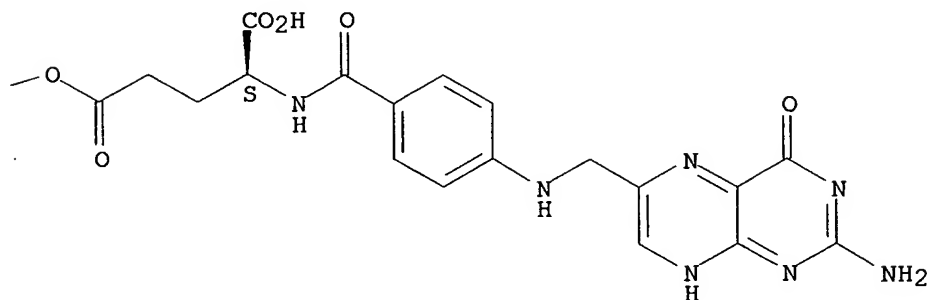
CN L-Glutamic acid, N-[4-[[[2-amino-1,4-dihydro-4-oxo-6-
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 sulfopropyl)acridinium-9-yl]carbonyl]oxy]phenyl]-19-oxo-3,6,9,12,15-
 penta-18-azanonadec-1-yl] ester, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

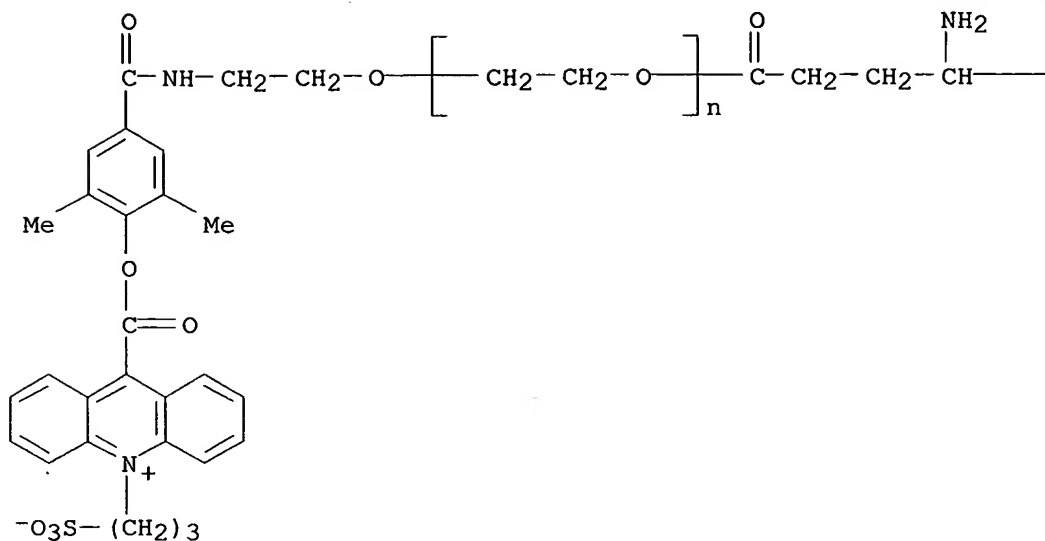


PAGE 1-B



RN 482648-48-6 HCAPLUS
 CN Poly(oxy-1,2-ethanediyl), .alpha.-[(4S)-4-amino-4-carboxy-1-oxobutyl]-
 .omega.-[2-[[3,5-dimethyl-4-[[[10-(3-sulfopropyl)acridinium-9-
 yl]carbonyl]oxy]benzoyl]amino]ethoxy]-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

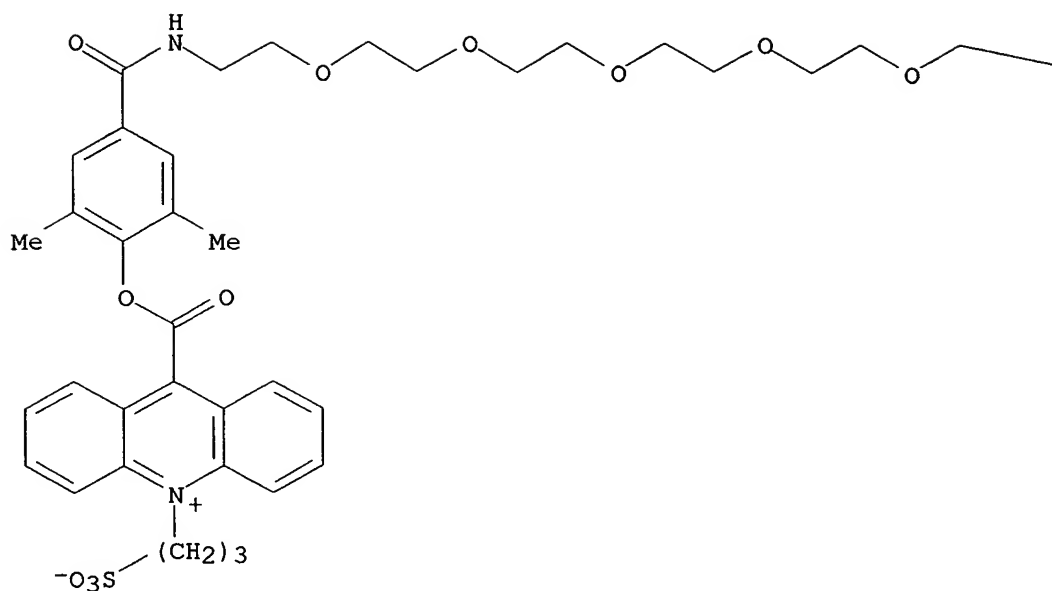
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RN 482648-49-7 HCAPLUS

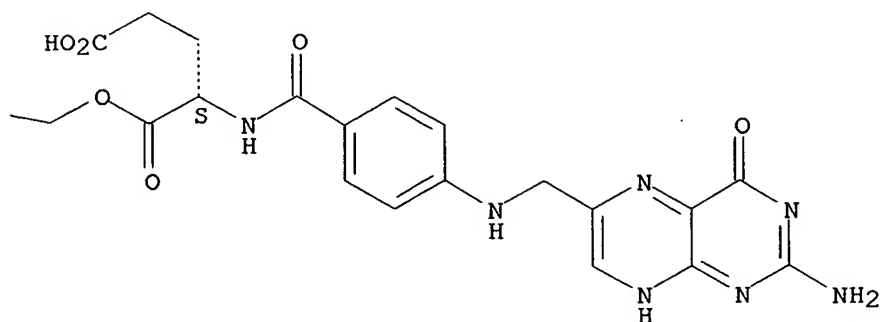
CN L-Glutamic acid, N-[4-[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl]-, 1-[19-[3,5-dimethyl-4-[[[10-(3-sulfopropyl)acridinium-9-yl]carbonyl]oxy]phenyl]-19-oxo-3,6,9,12,15-pentaoxa-18-azanonadec-1-yl] ester, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 482648-50-0 HCAPLUS

CN L-Glutamic acid, 1-[19-[3,5-dimethyl-4-[[[10-(3-sulfopropyl)acridinium-9-yl]carbonyl]oxy]phenyl]-19-oxo-3,6,9,12,15-pentaoxa-18-azanonadec-1-yl] ester, inner salt (9CI) (CA INDEX NAME)

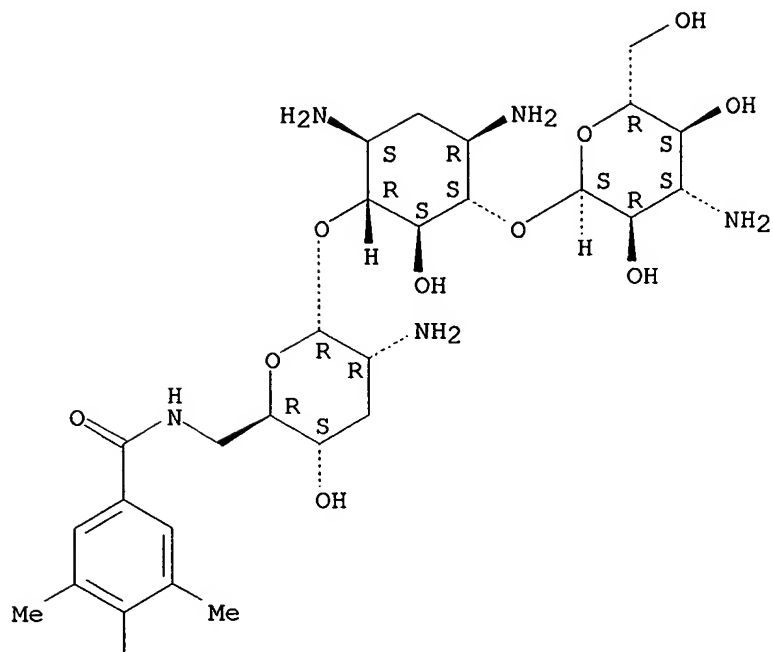
Absolute stereochemistry.

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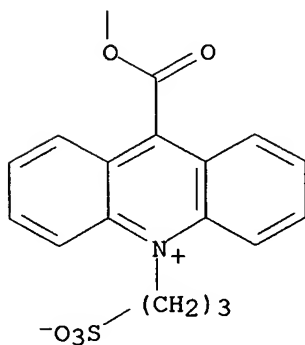
RN 482646-31-1 HCAFL05
 CN D-Streptamine, O-3-amino-3-deoxy-.alpha.-D-glucopyranosyl-(1.fwdarw.6)-O-
 [2-amino-2,3,6-trideoxy-6-[[[3,5-dimethyl-4-[[[10-(3-sulfopropyl)acridinium-
 9-yl]carbonyl]oxy]benzoyl]amino]-.alpha.-D-ribo-hexopyranosyl-
 (1.fwdarw.4)]-2-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

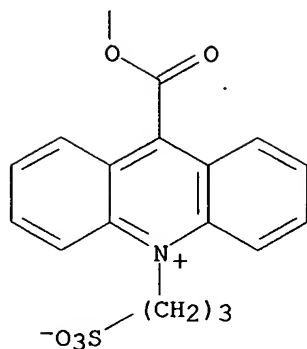


RN 482648-52-2 HCAPLUS
 CN D-Streptamine, O-3-amino-3-deoxy-.alpha.-D-glucopyranosyl-(1.fwdarw.6)-O-[2-amino-2,3,6-trideoxy-6-[[25-[3,5-dimethyl-4-[[[10-(3-sulfopropyl)acridinium-9-yl]carbonyl]oxy]phenyl]-1,5,25-trioxo-6,9,12,15,18,21-hexaoxa-24-azapentacos-1-yl]amino]-.alpha.-D-ribo-hexopyranosyl-(1.fwdarw.4)]-2-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

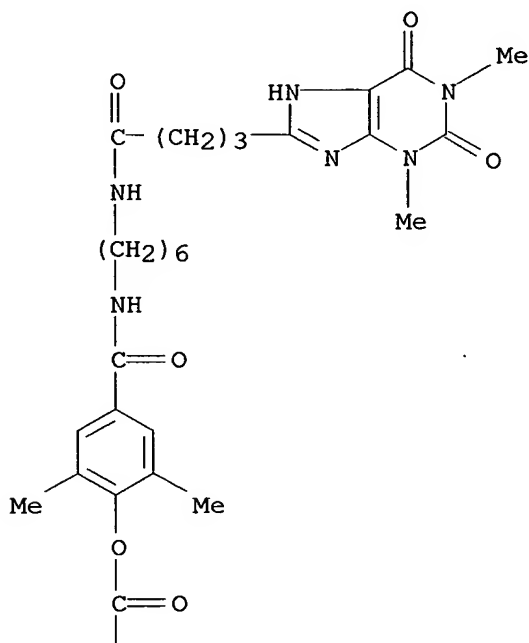
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PAGE 2-A

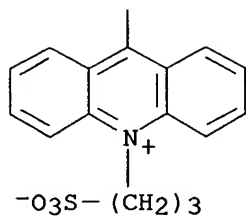


RN 482648-53-3 HCAPLUS
 CN Acridinium, 9-[[2,6-dimethyl-4-[[[6-[[1-oxo-4-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)butyl]amino]hexyl]amino]carbonyl]phenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

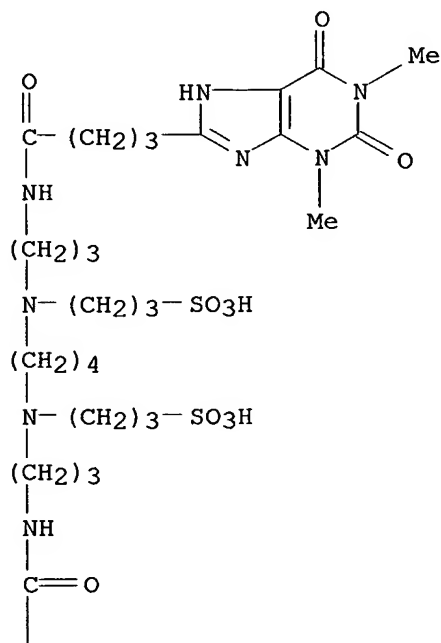


PAGE 2-A

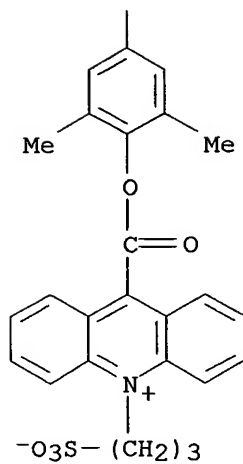


RN 482648-54-4 HCAPLUS
 CN Acridinium, 9-[[4-[1,16-dioxo-6,11-bis(3-sulfopropyl)-19-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)-2,6,11,15-tetraazanonadec-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI)
 (CA INDEX NAME)

PAGE 1-A

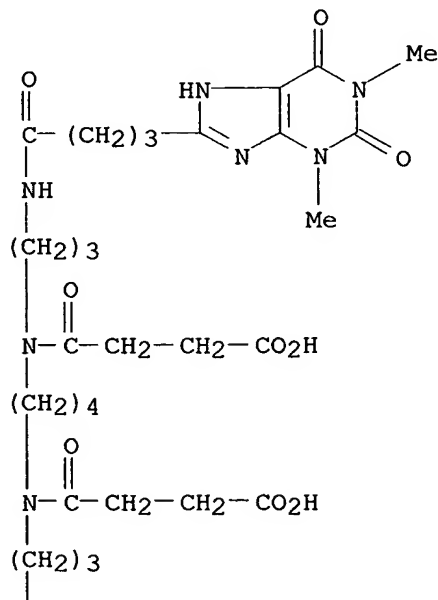


PAGE 2-A

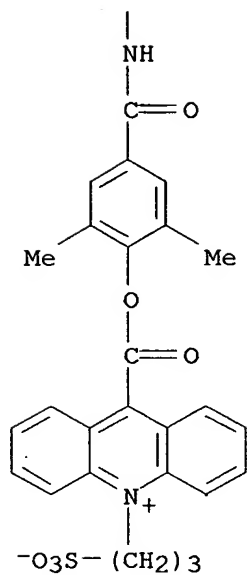


RN 482648-56-6 HCAPLUS
 CN Acridinium, 9-[[4-[6,11-bis(3-carboxy-1-oxopropyl)-1,16-dioxo-19-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)-2,6,11,15-tetraazonadec-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI)
 (CA INDEX NAME)

PAGE 1-A

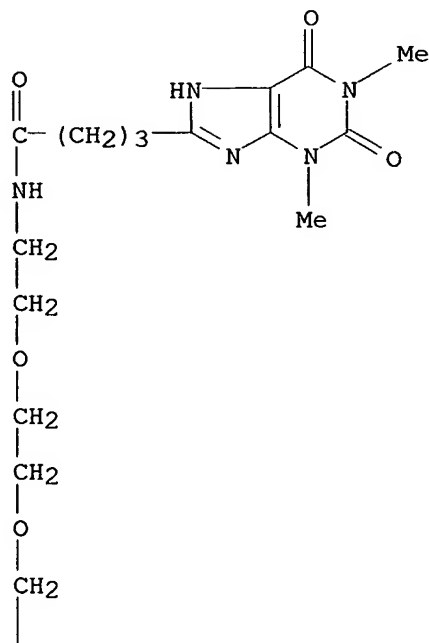


PAGE 2-A

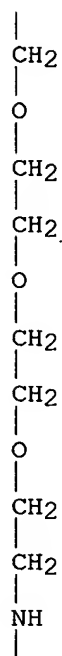


RN 482648-57-7 HCAPLUS
 CN Acridinium, 9-[[4-[[1,21-dioxo-24-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)-5,8,11,14,17-pentaoxa-2,20-diazatetracos-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

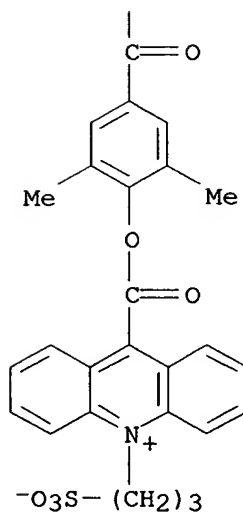
PAGE 1-A



PAGE 2-A



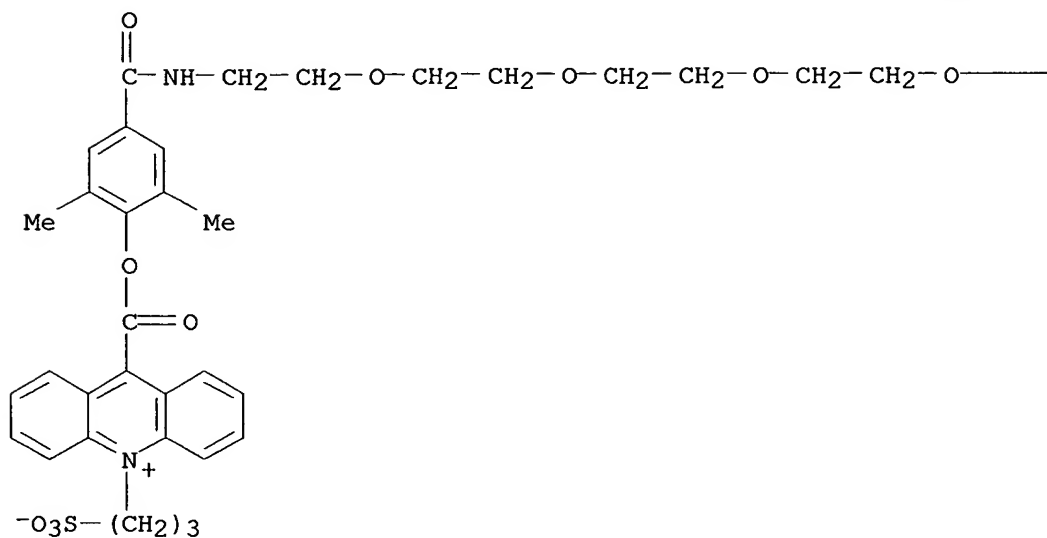
PAGE 3-A



IT **482648-39-5P 482648-44-2P 482648-55-5P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (acridinium ester labels having hydrophilic modifiers)
 RN 482648-39-5 HCAPLUS

CN Acridinium, 9-[[4-(19-amino-1-oxo-5,8,11,14,17-pentaoxa-2-azanonadec-1-yl)-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



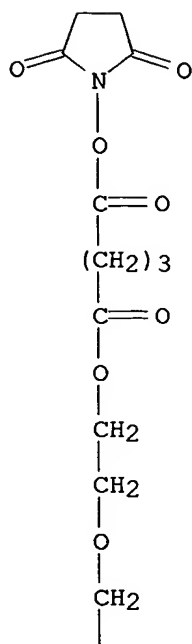
PAGE 1-B

$-CH_2-CH_2-O-CH_2-CH_2-NH_2$

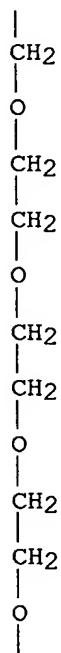
RN 482648-44-2 HCAPLUS

CN Acridinium, 9-[[4-[25-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1,21,25-trioxo-5,8,11,14,17,20-hexaoxa-2-azapentacos-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

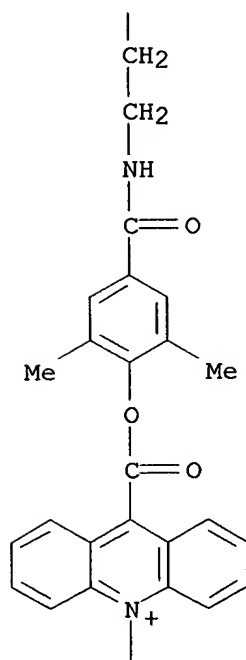
PAGE 1-A



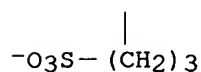
PAGE 2-A



PAGE 3-A

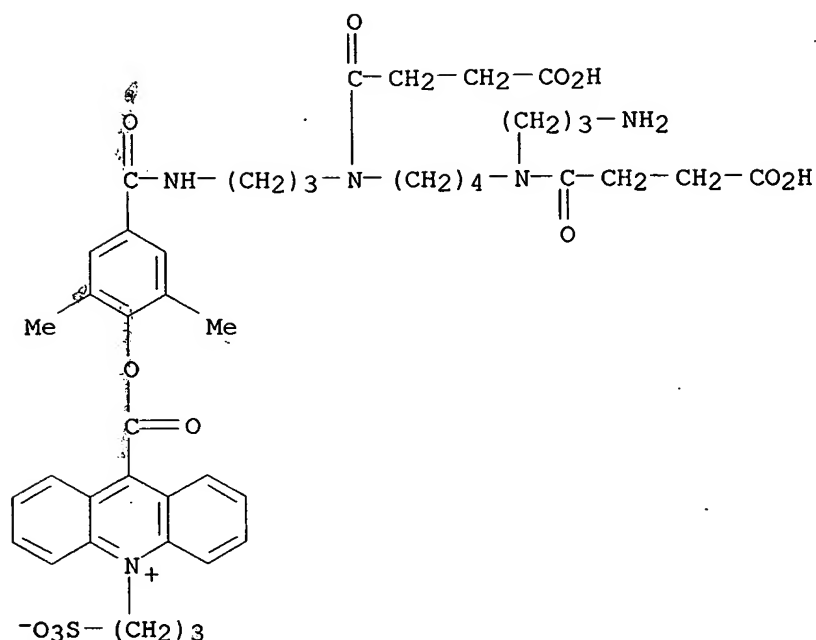


PAGE 4-A



RN 482648-55-5 HCAPLUS

CN Acridinium, 9-[[4-[[[3-[[4-[(3-aminopropyl)(3-carboxy-1-oxopropyl)amino]butyl](3-carboxy-1-oxopropyl)amino]propyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:256584 HCAPLUS

DOCUMENT NUMBER: 136:291356

TITLE: Novel branched linkers and their use for conjugate production

INVENTOR(S): Andres, Herbert; Josel, Hans-Peter; Hoess, Eva; Herrmann, Rupert; Von Der Eltz, Herbert

PATENT ASSIGNEE(S): Roche Diagnostics G.m.b.H., Germany; F. Hoffmann-La Roche A.-G.

SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2002027315 | A2 | 20020404 | WO 2001-EP11118 | 20010926 |
| WO 2002027315 | A3 | 20020711 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |

DE 10048417 A1 20020411 DE 2000-10048417 20000929

PRIORITY APPLN. INFO.: DE 2000-10048417 A 20000929

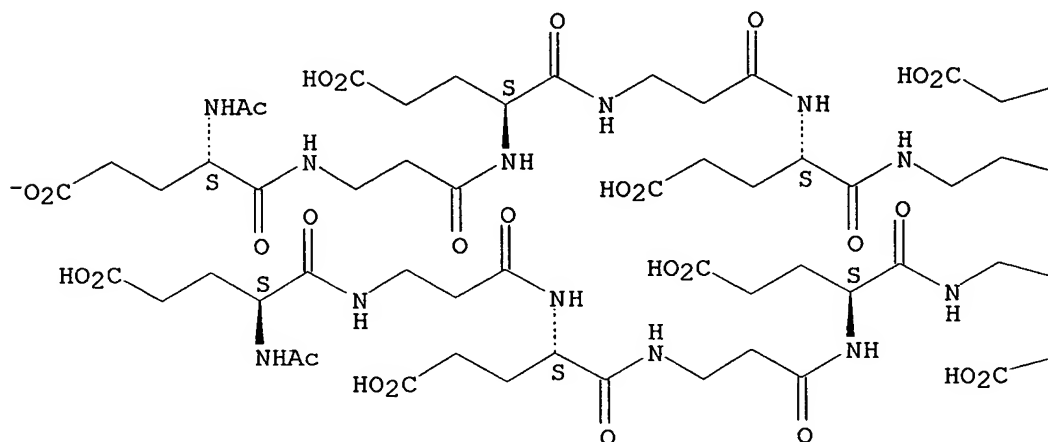
AB The present invention concerns new compds. comprising a branched linker

IT 406207-47-4P

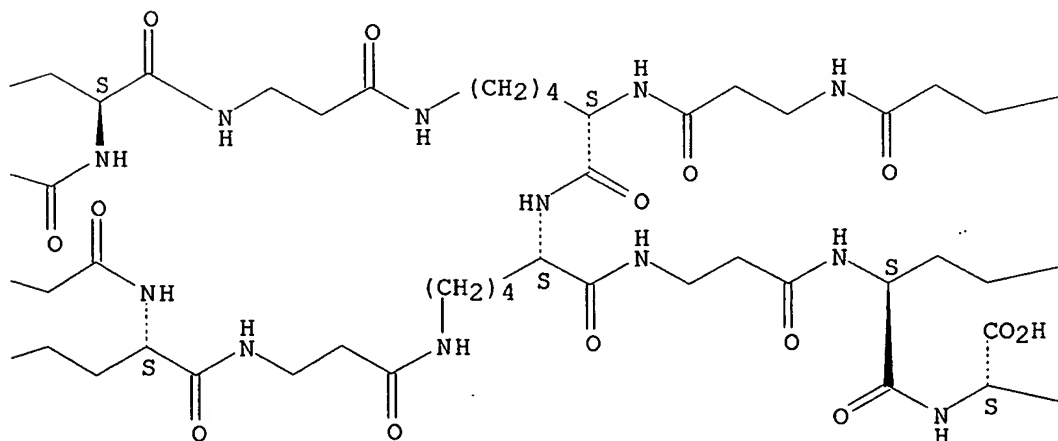
RN 406207-47-4 HCAPLUS

CN L-Lysine, N-[3-[4-[[(10-methylacridinium-9-yl) carbonyl]oxy]phenyl]-1-oxopropyl]-.beta.-alanyl-N6-(N-acetyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl)-L-lysyl-N6-(N-acetyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl-L-.alpha.-glutamyl-.beta.-alanyl)-L-lysyl-.beta.-alanyl-L-.alpha.-glutamyl-, inner salt (9CI) (CA INDEX NAME)

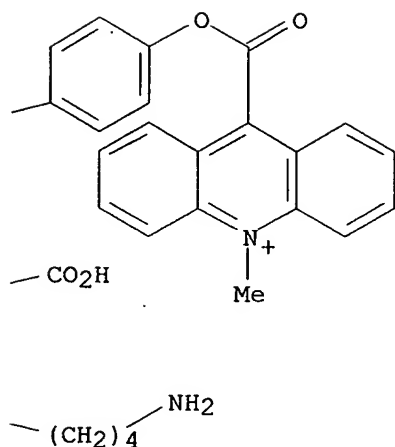
PAGE 1-A



PAGE 1-B



PAGE 1-C



L10 ANSWER 3 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:101348 HCAPLUS

DOCUMENT NUMBER: 134:159459

TITLE: **Chemiluminescent** substrates of hydrolytic enzymes such as phosphatases

INVENTOR(S): Jiang, Qingping; Natrajan, Anand; Sharpe, David J.; Wong, Wen-jee; Law, Say-jong

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

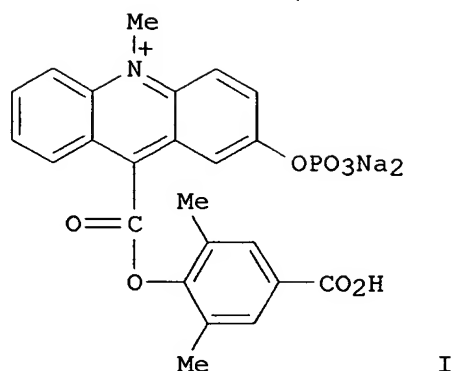
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2001009372 | A1 | 20010208 | WO 2000-US20429 | 20000727 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1203091 | A1 | 20020508 | EP 2000-950764 | 20000727 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |

PRIORITY APPLN. INFO.: US 1999-146648P P 19990730

WO 2000-US20429 W 20000727

OTHER SOURCE(S): MARPAT 134:159459

GI



AB **Chemiluminescent** substrates of hydrolytic enzymes are disclosed having the general Formula Lumi-M-P, where Lumi is a **chemiluminescent** moiety capable of producing light (a) by itself, (b) with MP attached and (c) with M attached, wherein the different properties of Lumi-M-P and Lumi-M allow them to be distinguished. Lumi includes, but is not limited to, acridinium compds. (e.g. acridinium esters, carboxyamides, thioesters, and oxime esters), reduced forms thereof (e.g. acridans), and spiroacridan compds. M is selected from oxygen, nitrogen and sulfur. P is a group that can be readily removed by hydrolytic enzymes to give Lumi-M and P. The hydrolytic enzyme can be phosphatase, glycosidase, peptidase, protease, esterase, sulfatase, and guanidinobenzoatase. Thus, 2-Phos-DMAE (I) is synthesized and shown to be an excellent substrate of hydrolytic alk. phosphatase to form 2-OH-DMAE. Both I and 2-OH-DMAE are **chemiluminescent**, but emit light at different emission maxima when they are treated with H₂O₂ in strong alk. soln. I emits a strong, visible blue light at λ_{max} 478 nm while 2-OH-DMAE emits a strong, visible orange light at λ_{max} 602 nm, thus resulting in a bathochromic shift of emission max. by 128 nm. One of the advantages in using **chemiluminescent** acridinium substrates like I to detect hydrolytic enzymes is that the products generated by the enzyme can be accumulated without undergoing significant decompn. during the enzymic reaction. In addn., under certain conditions the **chemiluminescence** from I is selectively and significantly suppressed, and thereby the overall signal differentiation of 2-OH-DMAE over I is improved. A heterogeneous immunoassay is also provided demonstrating I utility as a substrate for the **chemiluminescent** detection of TSH in human serum.

IT **324762-34-7P 324762-52-9P 324762-58-5P**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(**chemiluminescent** substrates of hydrolytic enzymes such as phosphatases)

RN 324762-34-7 HCAPLUS

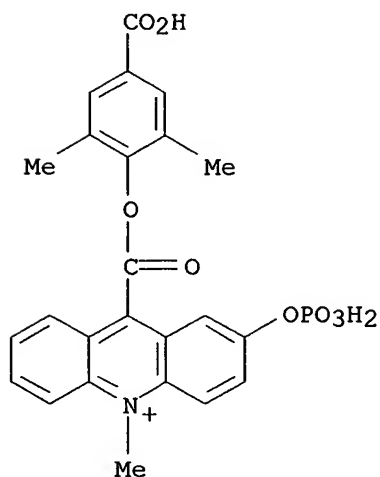
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-2-(phosphonooxy)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX

NAME)

CM 1

CRN 324762-33-6

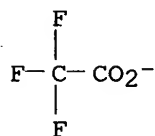
CMF C24 H21 N O8 P



CM 2

CRN 14477-72-6

CMF C2 F3 O2



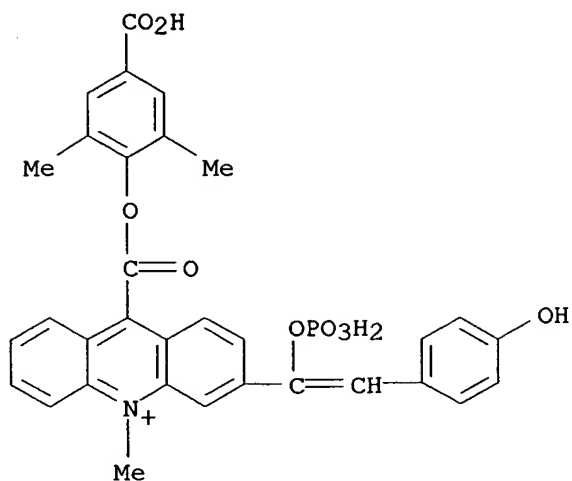
RN 324762-52-9 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-hydroxyphenyl)-1-(phosphonooxy)ethenyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 324762-51-8

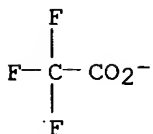
CMF C32 H27 N O9 P



CM 2

CRN 14477-72-6

CMF C2 F3 O2



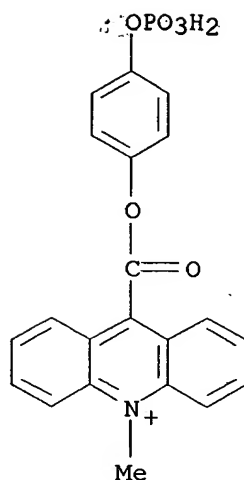
RN 324762-58-5 HCAPLUS

CN Acridinium, 10-methyl-9-[[4-(phosphonooxy)phenoxy]carbonyl]-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 324762-57-4

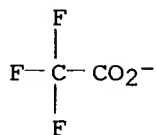
CMF C21 H17 N O6 P



CM 2

CRN 14477-72-6

CMF C2 F3 O2

IT **324762-59-6P**

RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(**chemiluminescent** substrates of hydrolytic enzymes such as phosphatases)

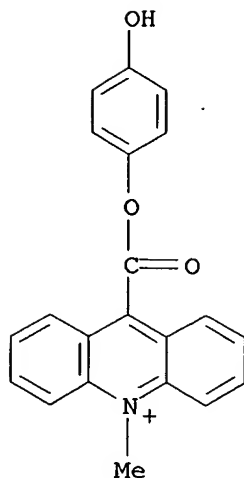
RN 324762-59-6 HCAPLUS

CN Acridinium, 9-[(4-hydroxyphenoxy)carbonyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 161006-16-2

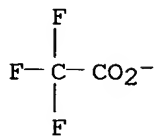
CMF C21 H16 N O3



CM 2

CRN 14477-72-6

CMF C2 F3 O2



IT 324762-35-8P 324762-43-8P 324762-44-9P

324762-46-1P 324762-48-3P 324762-54-1P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(**chemiluminescent** substrates of hydrolytic enzymes such as phosphatases)

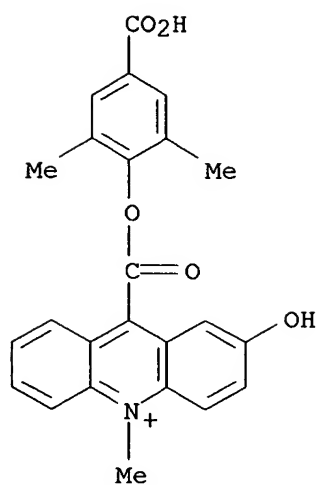
RN 324762-35-8 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-hydroxy-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 259169-42-1

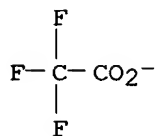
CMF C24 H20 N O5



CM 2

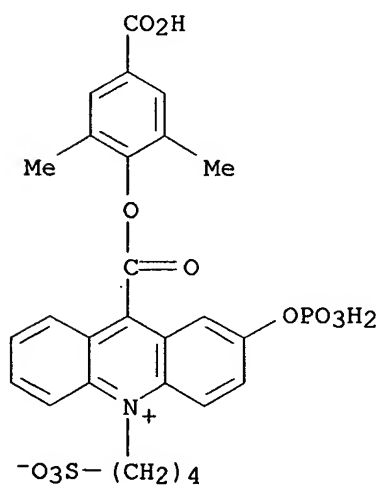
CRN 14477-72-6

CMF C2 F3 O2



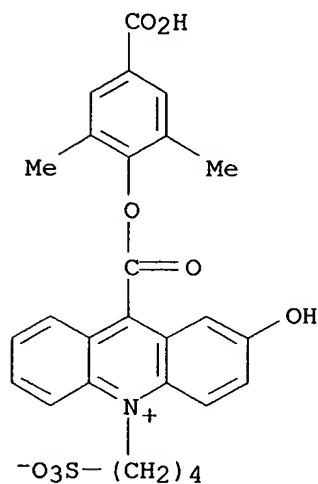
RN 324762-43-8 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-(phosphonooxy)-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



RN 324762-44-9 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-hydroxy-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



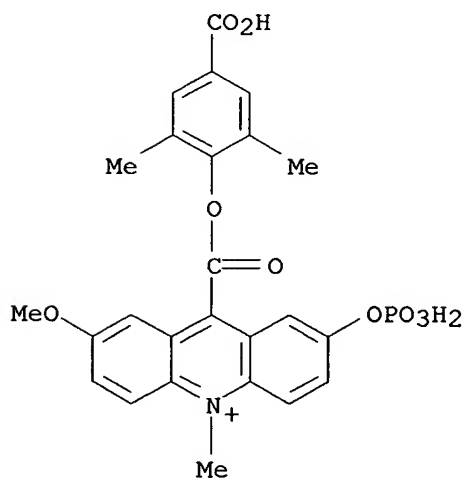
RN 324762-46-1 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-methoxy-10-methyl-7-(phosphonoxy)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

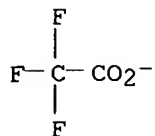
CRN 324762-45-0

CMF C25 H23 N O9 P



CM 2

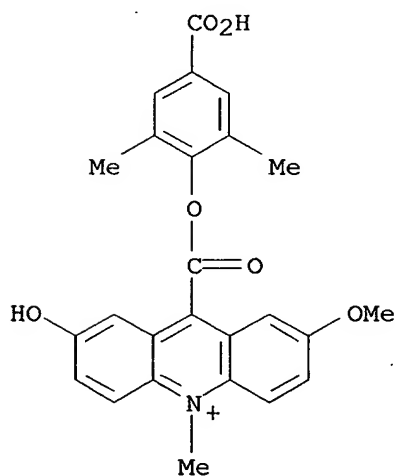
CRN 14477-72-6
CMF C2 F3 O2



RN 324762-48-3 HCAPLUS
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-hydroxy-7-methoxy-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

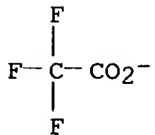
CM 1

CRN 324762-47-2
CMF C25 H22 N O6



CM 2

CRN 14477-72-6
CMF C2 F3 O2



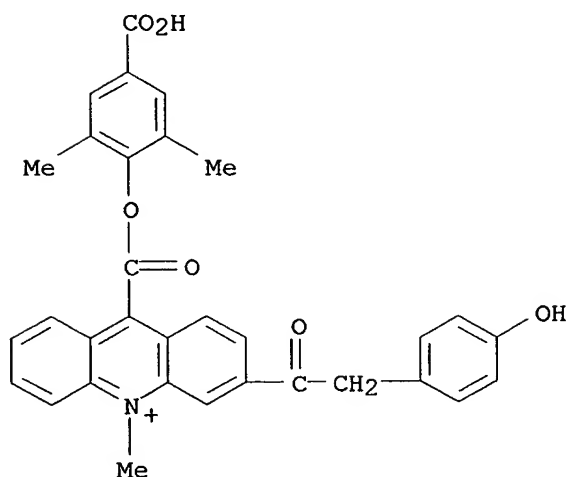
RN 324762-54-1 HCAPLUS
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[(4-

hydroxyphenyl)acetyl]-10-methyl-, salt with trifluoroacetic acid (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 324762-53-0

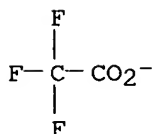
CMF C32 H26 N O6



CM 2

CRN 14477-72-6

CMF C2 F3 O2



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:133665 HCAPLUS

DOCUMENT NUMBER: 132:191423

TITLE: Synthesis of near infrared **chemiluminescent** acridinium compounds and their application for labeling proteins and nucleotides

INVENTOR(S): Natrajan, Anand; Jiang, Qingping; Sharpe, David; Law, Say-Jong

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|-------------|
| WO 2000009487 | A1 | 20000224 | WO 1999-US18076 | 19990810 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 9954739 | A1 | 20000306 | AU 1999-54739 | 19990810 |
| EP 1104405 | A1 | 20010606 | EP 1999-941005 | 19990810 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 6355803 | B1 | 20020312 | US 1999-371489 | 19990810 |
| JP 2002522530 | T2 | 20020723 | JP 2000-564941 | 19990810 |
| US 2002076823 | A1 | 20020620 | US 2001-6421 | 20011206 |
| PRIORITY APPLN. INFO.: | | | US 1998-96073P | P 19980811 |
| | | | US 1999-371489 | A3 19990810 |
| | | | WO 1999-US18076 | W 19990810 |
| AB Our results identify two sets of necessary and sufficient criteria for observing long-wavelength emission from acridinium compds.: Set A: (a) the creation of an extended conjugation system by the attachment of appropriate functional groups on the acridinium nucleus (electronic requirement); (b) coplanarity of the attached functional group and the acridone moiety during light emission (geometry requirement); (c) said functional group must consist of at least one arom. ring and one electron-donating atom or group with an extra pair of electrons which can readily delocalize into the extended .pi. system to which the heteroatom is directly attached or built into, and establish stable extended resonance with the electron-withdrawing carbonyl moiety of the light emitting acridone. Such electron-donating atom or group that exists in the form of an anion has particularly strong effect to further the bathochromic shift of the emission wavelength. Set B: (a) A direct attachment at one or more of positions C-2, C-4, C-5, or C-7 of the acridinium nucleus, of electron-donating atoms or groups having extra pair(s) of electrons. The electron-donating entities can be the same or different if more than one electron-donating entity is used. Such electron-donating atom or group that exists in the form of an anion has particularly strong effect to further the bathochromic shift of the emission wavelength. For mols. for which the above criteria are met such as LEAE, 3-HS-DMAE, and 2-hydroxy-DMAE long wavelength-emission exceeding 500 nm and reaching into NIR region is expected and obsd. Preferably, the utility of an NIR-AC of comparable quantum yield as the conventional acridinium compds. goes hand-in-hand with the employment of a luminescence detector of good to excellent detection efficiency. To achieve efficient NIR signal detection and facilitate the performing of diagnostic assays, a further objective of the present invention is the advance of a concept and the realization of substituting a state-of-the-art charge-coupled device (CCD) detector for the red-insensitive photomultiplier tube (PMT) in a conventional fully or semi-automatic analyzer such as MLA-II of Chiron | | | | |

Diagnostics, Walpole, MA.

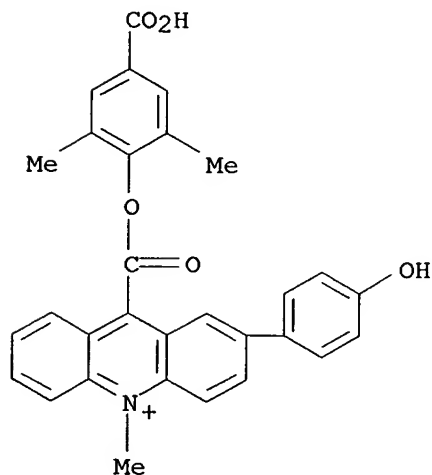
IT 259169-37-4P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(2-HP-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-37-4 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-(4-hydroxyphenyl)-10-methyl- (9CI) (CA INDEX NAME)



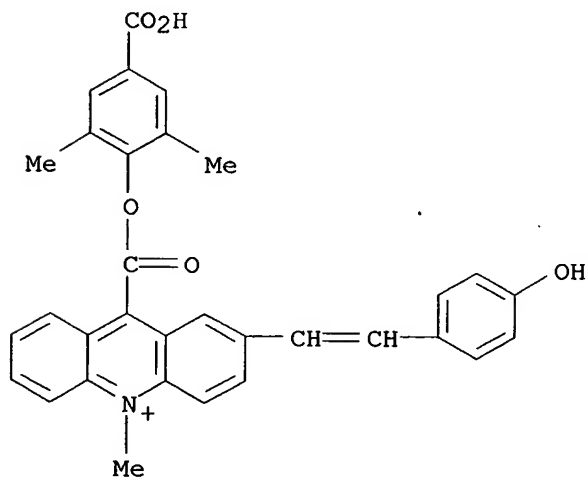
IT 259169-25-0P

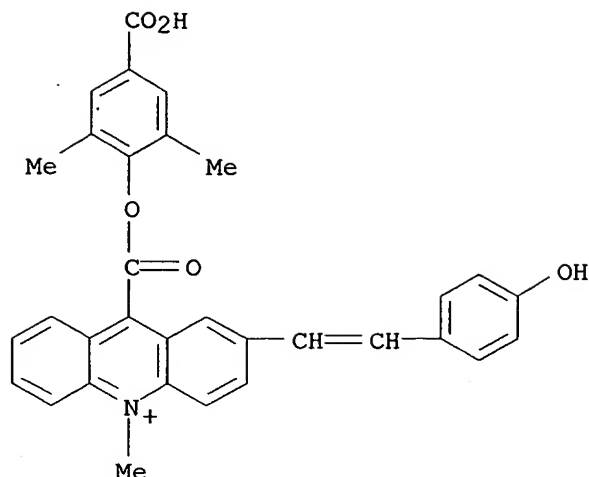
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(2-HS-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-25-0 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-[2-(4-hydroxyphenyl)ethenyl]-10-methyl- (9CI) (CA INDEX NAME)



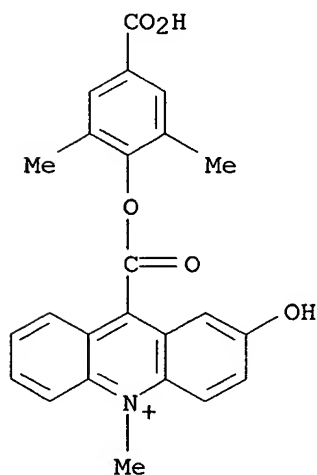


IT 259169-42-1P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(2-OH-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-42-1 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-hydroxy-10-methyl- (9CI) (CA INDEX NAME)

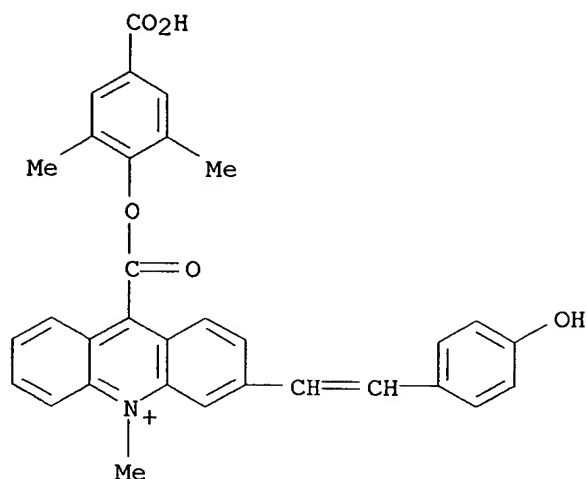


IT 259169-10-3P

RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(3-HS-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-10-3 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-hydroxyphenyl)ethenyl]-10-methyl- (9CI) (CA INDEX NAME)



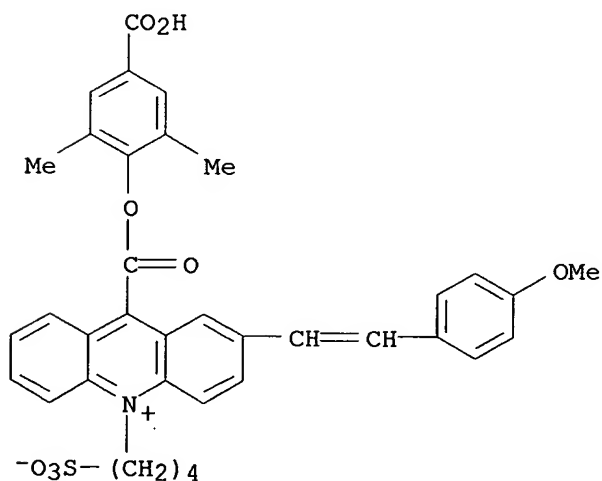
IT **259169-36-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(NSB-2-MS-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-36-3 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-[2-(4-methoxyphenyl)ethenyl]-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



IT **259169-19-2P**

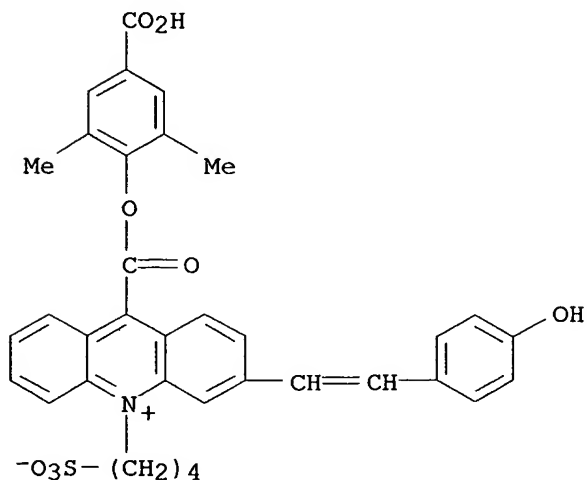
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(NSB-3-HS-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and

nucleotides)

RN 259169-19-2 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-hydroxyphenyl)ethenyl]-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



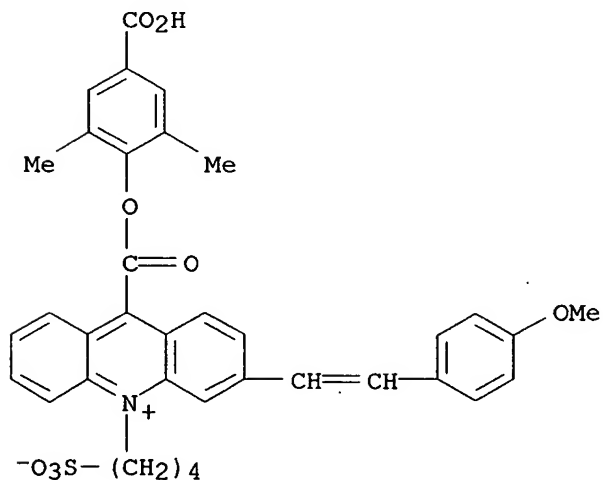
IT 259169-24-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

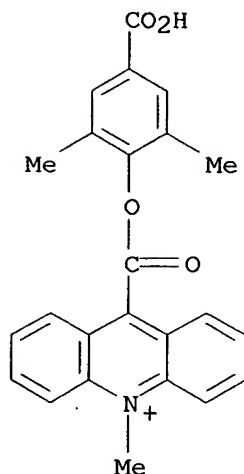
(NSB-3-MS-DMAE; synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-24-9 HCAPLUS

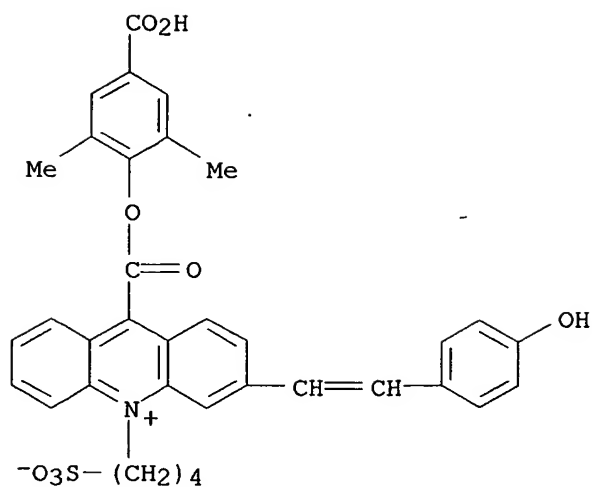
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-methoxyphenyl)ethenyl]-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



IT **148794-24-5D**, DMAE, conjugate with vancomycin A probe
RL: ANT (Analyte); ANST (Analytical study)
(Vanco B synthetic target 459.23, vancomycin B resistance gene;
synthesis of near IR **chemiluminescent** acridinium compds. and
application for labeling proteins and nucleotides)
RN 148794-24-5 HCAPLUS
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl- (9CI)
(CA INDEX NAME)

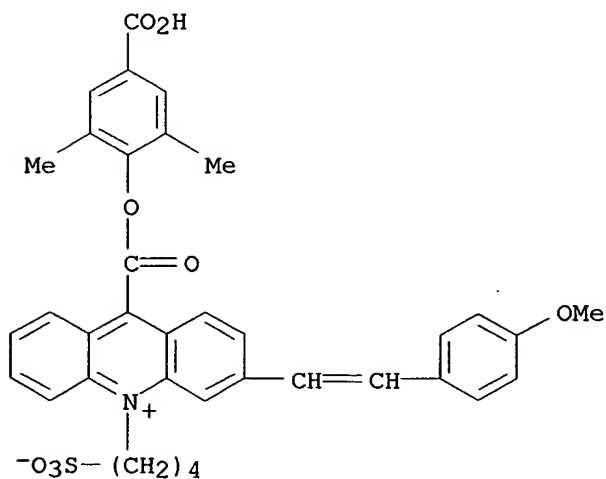


IT **259169-19-2DP**, conjugates with BSA and anti-TSH
259169-24-9DP, conjugates with BSA and anti-TSH
RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study);
PREP (Preparation)
(synthesis of near IR **chemiluminescent** acridinium compds. and
application for labeling proteins and nucleotides)
RN 259169-19-2 HCAPLUS
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-hydroxyphenyl)ethenyl]-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



RN 259169-24-9 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[2-(4-methoxyphenyl)ethenyl]-10-(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)



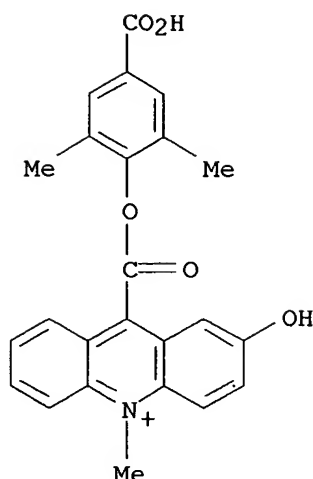
IT 259169-42-1DP, conjugate with Vancomycin A probe

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of near IR **chemiluminescent** acridinium compds. and application for labeling proteins and nucleotides)

RN 259169-42-1 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-hydroxy-10-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 51 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:317213 HCAPLUS

DOCUMENT NUMBER: 130:335007

TITLE: Extended dynamic range assays using at least two labeled probes for different target regions on an analyte

INVENTOR(S): Nelson, Norman C.

PATENT ASSIGNEE(S): Gen-Probe Incorporated, USA

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 9923490 | A1 | 19990514 | WO 1998-US23088 | 19981030 |
| W: AU, CA, JP, KR | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 6180340 | B1 | 20010130 | US 1997-962033 | 19971031 |
| CA 2305415 | AA | 19990415 | CA 1998-2305415 | 19981030 |
| AU 9912918 | A1 | 19990524 | AU 1999-12918 | 19981030 |
| AU 741568 | B2 | 20011206 | | |
| EP 1027604 | A1 | 20000816 | EP 1998-956381 | 19981030 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE | | | | |
| JP 2002508504 | T2 | 20020319 | JP 2000-519300 | 19981030 |
| US 6350579 | B1 | 20020226 | US 2000-649636 | 20000828 |

PRIORITY APPLN. INFO.: US 1997-962033 A 19971031
WO 1998-US23088 W 19981030

AB Methods of detecting and/or quantifying an analyte in a single sample by using at least two labeled probes that specifically bind to different target regions of an analyte, and are labeled with labels that are distinguishable and/or present at different specific activities, are

disclosed. Compns. comprising at least two labeled probes that specifically bind to different target regions of the same analyte and are labeled with labels that are distinguishable and/or present at different specific activities are disclosed. 1-Methyl-m-difluoroacridinium ester, 1-methylacridinium ester, and o-methoxy(cinnamyl)acridinium ester were shown to be distinguishable under conditions that replicate those of analyte detection using **chemiluminescence**. The three labels were used at a specific activity of 108, 106, and 104, resp.

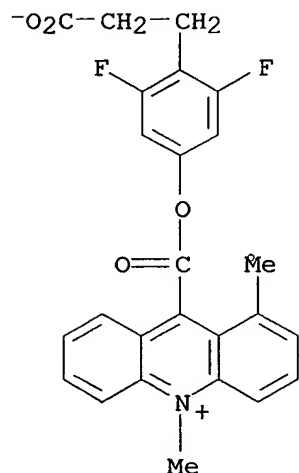
IT 224169-61-3 224169-63-5 224169-64-6

RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)

(as detectable label; extended dynamic range assays using at least two labeled probes for different target regions on an analyte)

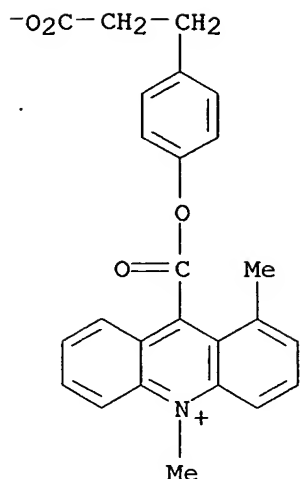
RN 224169-61-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-1,10-dimethyl-, inner salt (9CI) (CA INDEX NAME)



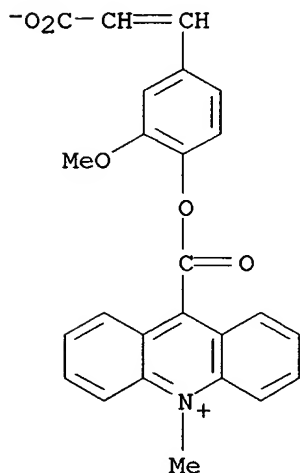
RN 224169-63-5 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-1,10-dimethyl-, inner salt (9CI) (CA INDEX NAME)



RN 224169-64-6 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethenyl)-2-methoxyphenoxy]carbonyl]-10-methyl-, inner salt (9CI) (CA INDEX NAME)



IT 224169-65-7DP, conjugates with oligonucleotide probe

224169-66-8DP, conjugates with oligonucleotide probe

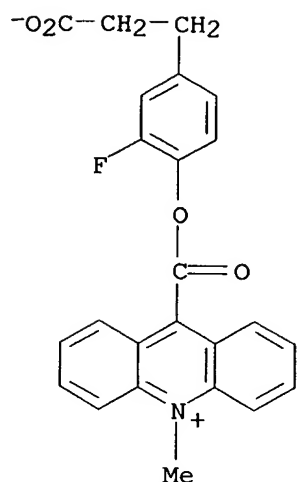
224169-67-9DP, conjugates with oligonucleotide probe

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

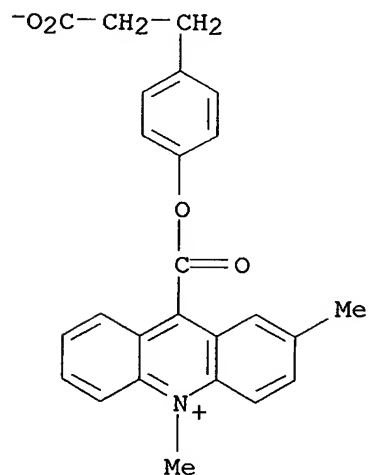
(for synthetic RNA oligomer detn.; extended dynamic range assays using at least two labeled probes for different target regions on an analyte)

RN 224169-65-7 HCAPLUS

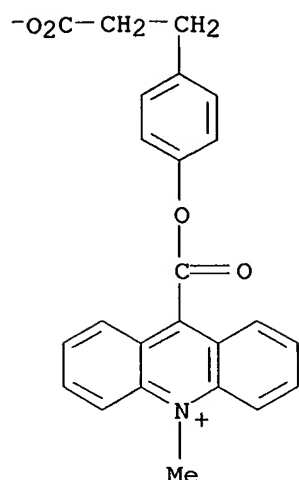
CN Acridinium, 9-[[4-(2-carboxyethyl)-2-fluorophenoxy]carbonyl]-10-methyl-, inner salt (9CI) (CA INDEX NAME)



RN 224169-66-8 HCAPLUS
CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-2,10-dimethyl-, inner salt (9CI) (CA INDEX NAME)



RN 224169-67-9 HCAPLUS
CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-10-methyl-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:183770 HCAPLUS

DOCUMENT NUMBER: 130:220167

TITLE: Long emission wavelength **chemiluminescent** ring-fused acridinium compounds and their use in test assays

INVENTOR(S): Law, Say-jong; Jiang, Qingping; Fischer, Walter; Unger, John T.; Krodell, Elizabeth K.; Xi, Jun

PATENT ASSIGNEE(S): Chiron Diagnostics Corporation, USA

SOURCE: U.S., 80 pp., Cont.-in-part of U.S. 5,395,752.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| US 5879894 | A | 19990309 | US 1994-308772 | 19940919 |
| US 5395752 | A | 19950307 | US 1993-35130 | 19930319 |
| AU 9455018 | A1 | 19940922 | AU 1994-55018 | 19940210 |
| AU 677259 | B2 | 19970417 | | |
| CA 2118891 | AA | 19940920 | CA 1994-2118891 | 19940311 |
| WO 9421823 | A1 | 19940929 | WO 1994-US3020 | 19940318 |
| W: PL | | | | |
| PL 178927 | B1 | 20000630 | PL 1994-306210 | 19940318 |
| JP 08320319 | A2 | 19961203 | JP 1994-50109 | 19940322 |
| US 5702887 | A | 19971230 | US 1994-340093 | 19941114 |

PRIORITY APPLN. INFO.: US 1993-35130 A2 19930319
WO 1994-US3020 W 19940318

AB The present invention relates to a new class of **chemiluminescent**, arom. ring-fused acridinium compds. (AFAC) which emit green or yellow light upon simple chem. treatments. This invention also relates to conjugates formed from AFAC and binding partners, e.g. biol. mols., and test assays utilizing the conjugates. The synthesis of

chemiluminescent reagents or conjugates for use in such methods as well as kits incorporating such reagents are also disclosed. Furthermore, the invention relates to test assays in which the detection and/or quantitation of two or more substances or analytes in a test sample can be carried out simultaneously due to the discernable and non-interfering light emission characteristics of two or more **chemiluminescent** conjugates. The assays have particular application in the field of clin. diagnostics.

IT 221057-47-2P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(long emission wavelength **chemiluminescent** ring-fused acridinium compds. and their use in test assays)

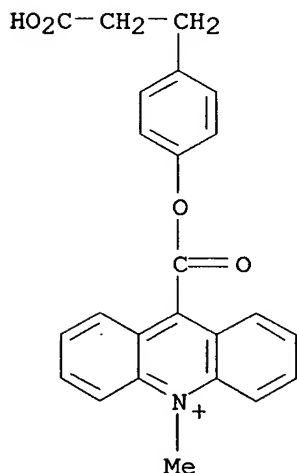
RN 221057-47-2 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-60-4

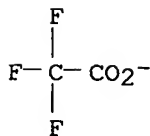
CMF C24 H20 N O4



CM 2

CRN 14477-72-6

CMF C2 F3 O2



REFERENCE COUNT:

63

THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:795185 HCAPLUS

DOCUMENT NUMBER: 130:35376

TITLE: **Chemiluminescent** energy transfer conjugates
and their uses as labels in binding assaysINVENTOR(S): Jiang, Qingping; Xi, Jun; Natrajan, Anand; Sharpe,
David; Baumann, Marcus; Hilfiker, Rolf; Schmidt,
Erika; Senn, Paul; Thommen, Fritz; Waldner, Adrian;
Alder, Alex; Law, Say-jong

PATENT ASSIGNEE(S): Chiron Diagnostics Corporation, USA; et al.

SOURCE: PCT Int. Appl., 104 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9854574 | A2 | 19981203 | WO 1998-IB831 | 19980529 |
| WO 9854574 | A3 | 19990304 | | |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| US 6165800 | A | 20001226 | US 1998-86003 | 19980527 |
| AU 9873472 | A1 | 19981230 | AU 1998-73472 | 19980529 |
| EP 988551 | A2 | 20000329 | EP 1998-920688 | 19980529 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 2002506518 | T2 | 20020226 | JP 1999-500420 | 19980529 |
| PRIORITY APPLN. INFO.: | | | US 1997-48159P | P 19970530 |
| | | | WO 1998-IB831 | W 19980529 |

OTHER SOURCE(S): MARPAT 130:35376

AB A new class of **chemiluminescent** acridinium or benzacridinium compds. forms an intramol. energy transfer conjugate (ETC) between the acridinium or benzacridinium compd. and a luminophor. A method of extending the emission wavelengths of acridinium or benzacridinium esters to further reduce or eliminate the emission spectral overlap between the parent polysubstituted aryl acridinium esters (DMAE) and benzacridinium esters (LEAE) is disclosed. The ETC's retain the unique desired properties of acridinium or benzacridinium compds. including complete light emission in very short period of time, monophasic emission spectrum, simplicity of triggering mechanism, ability of labeling the biol. mols. of interest to form a tracer, and good stability. Addnl., the range of the emission spectrum of an acridinium or benzacridinium compd. can now be shifted at will and at longer leap through the choice of a luminophor as the integral part of an ETC mol. **Chemiluminescent** labeled conjugates comprise an acridinium or benzacridinium moiety covalently attached to a luminophor via a spacer, said moiety further conjugated to a biol. mol. of interest, wherein said spacer is of an appropriate length to

allow the excited species generated from said moiety to transfer energy efficiently to said luminophor, resulting in the emission of light in the spectral region of said luminophor. The conjugates are used in binding assays and test kits; methods for prepn. of the conjugates are presented.

IT **216670-03-0P**

RL: ARG (Analytical reagent use); IMF (Industrial manufacture); ANST (Analytical study); PREP (Preparation); USES (Uses)

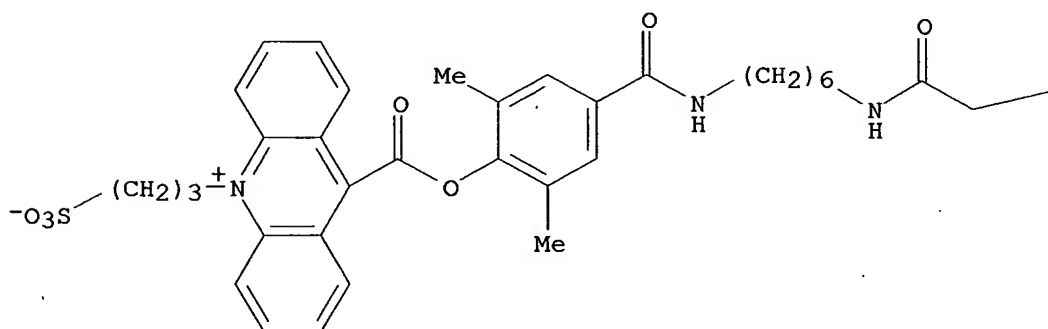
(conjugate; prepn. of **chemiluminescent** energy transfer conjugates for labels in binding assays)

RN 216670-03-0 HCAPLUS

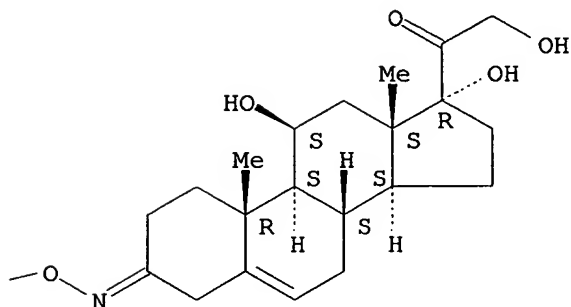
CN Acridinium, 9-[[2,6-dimethyl-4-[[[6-[[[(11.beta.)-11,17,21-trihydroxy-20-oxopregn-5-en-3-ylidene]amino]oxy]acetyl]amino]hexyl]amino]carbonyl]phenoxyl]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



IT **216667-69-5P 216667-78-6P 216668-22-3P**

216668-30-3P 216668-38-1P 216668-46-1P

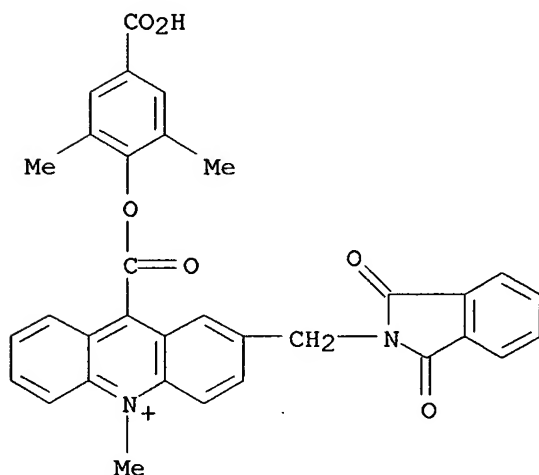
216669-79-3P 216669-87-3P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of **chemiluminescent** energy transfer conjugates for labels in binding assays)

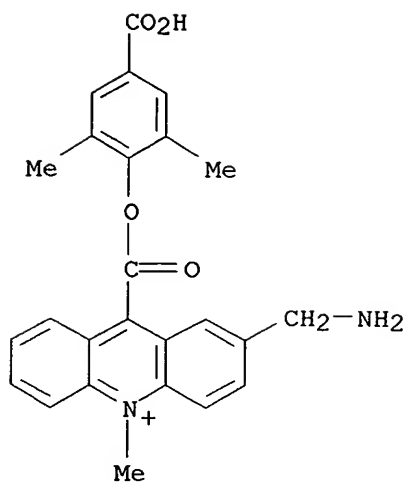
RN 216667-69-5 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

● Br⁻

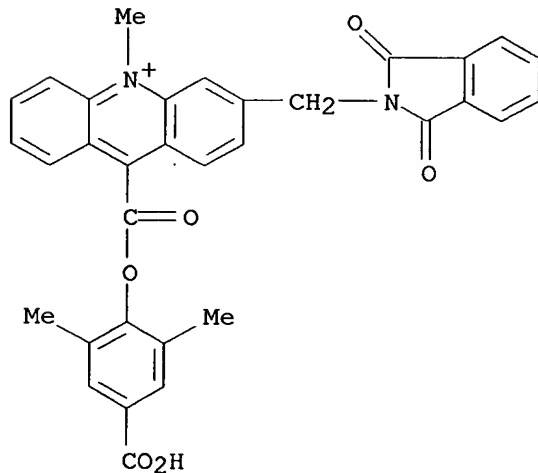
RN 216667-78-6 HCAPLUS

CN Acridinium, 2-(aminomethyl)-9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



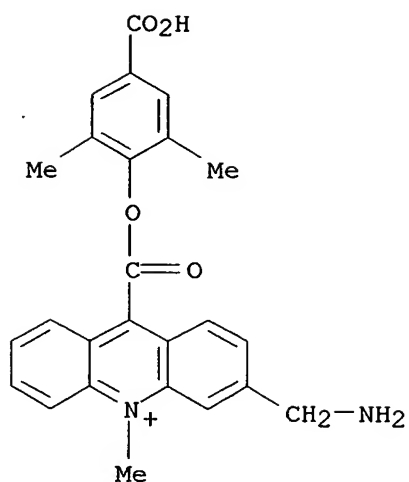
● Br⁻

RN 216668-22-3 HCAPLUS
 CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-3-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 216668-30-3 HCAPLUS
 CN Acridinium, 3-(aminomethyl)-9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

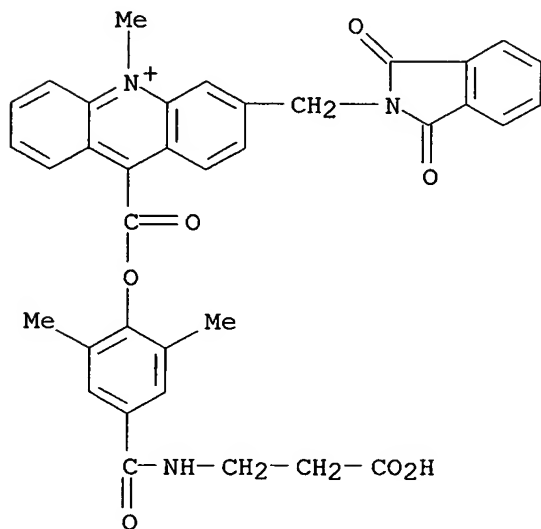
RN 216668-38-1 HCAPLUS

CN Acridinium, 9-[[4-[[(2-carboxyethyl) amino] carbonyl]-2,6-dimethylphenoxy]carbonyl]-3-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 216668-37-0

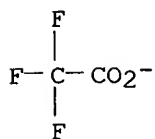
CMF C36 H30 N3 O7



CM 2

CRN 14477-72-6

CMF C2 F3 O2



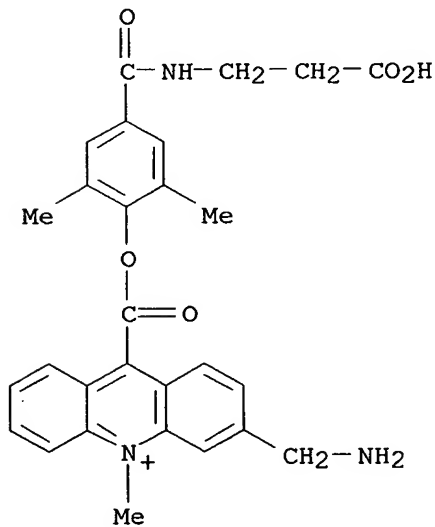
RN 216668-46-1 HCAPLUS

CN Acridinium, 3-(aminomethyl)-9-[[4-[[[(2-carboxyethyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, salt with trifluoroacetic acid (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 216668-45-0

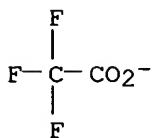
CMF C28 H28 N3 O5

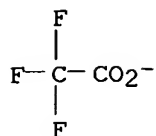


CM 2

CRN 14477-72-6

CMF C2 F3 O2





RN 216669-79-3 HCAPLUS

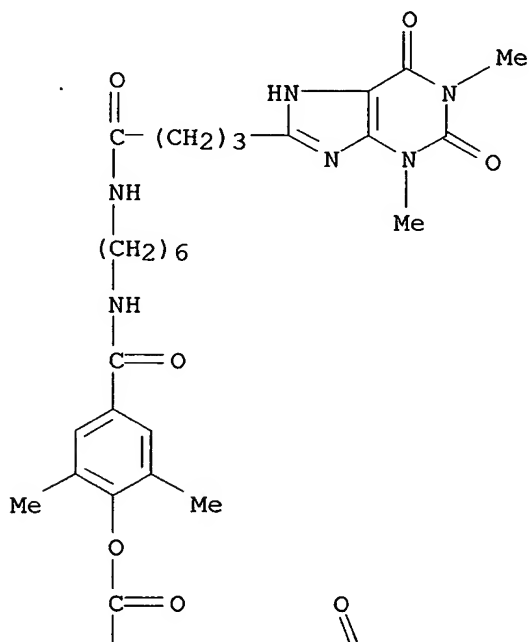
CN Acridinium, 2-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-9-[[2,6-dimethyl-4-[[[6-[[1-oxo-4-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)butyl]amino]hexyl]amino]carbonyl]phenoxy]carbonyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 216669-78-2

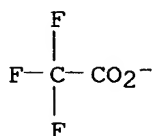
CMF C50 H51 N8 O8

PAGE 1-A



The chemical structure shows a fluorenyl cation core. The central nitrogen atom is positively charged (N⁺) and is bonded to a methyl group (Me) below it. The 2-position of the fluorene system is substituted with a (2-methyl-1H-indol-3-yl)methyl group, represented as -CH₂- attached to the 3-position of an indole ring. The indole ring has a methyl group at its 2-position and a double bond at the 3-position.

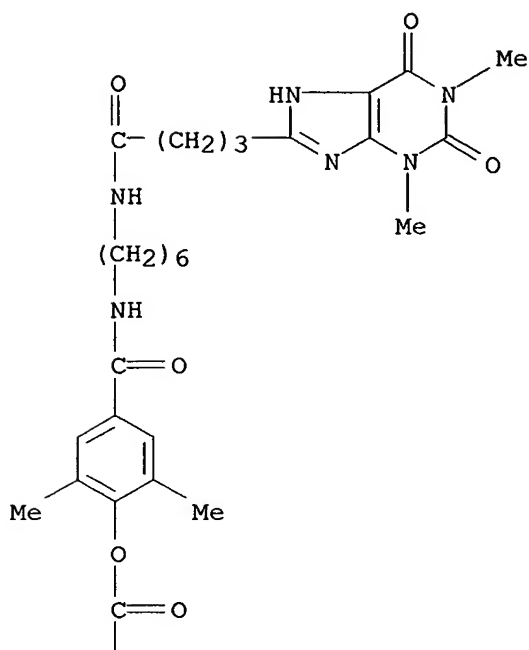
CMF C2 F3 02



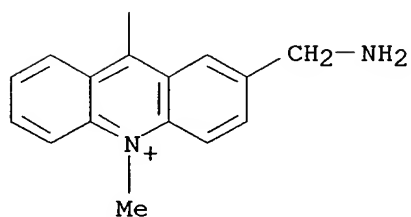
Acridinium, 2-(aminomethyl)-9-[[[2,6-dimethyl-4-[[[6-[[1-oxo-4-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)butyl]amino]hexyl]amino]carbonyl]phenoxy]carbonyl]-10-methyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CMF C42 H49 N8 O6

PAGE 1-A



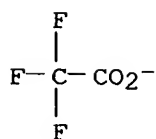
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



IT 216669-95-3P

RL: ARG (Analytical reagent use); IMF (Industrial manufacture); ANST (Analytical study); PREP (Preparation); USES (Uses)

(prepn. of **chemiluminescent** energy transfer conjugates for
labels in binding assays)

RN 216669-95-3 HCAPLUS

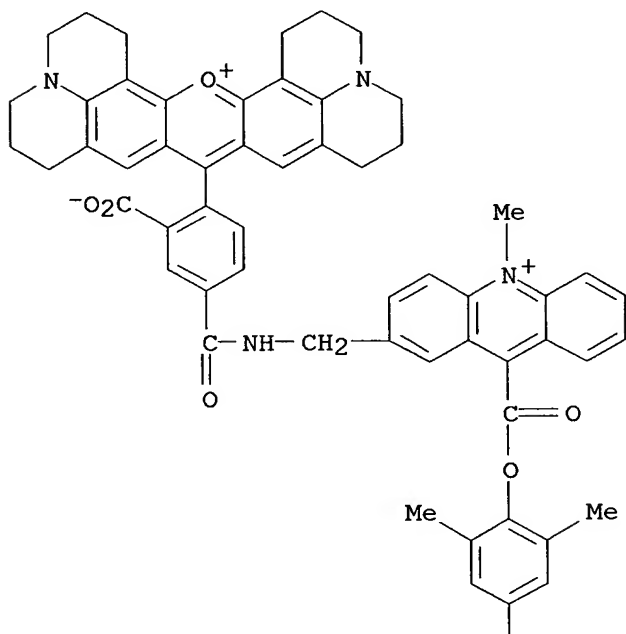
CN 1H, 5H, 11H, 15H-Xantheno[2,3,4-ij:5,6,7-i'j']diquinolizin-18-ium,
9-[2-carboxy-4-[[[9-[[2,6-dimethyl-4-[[[6-[[1-oxo-4-(2,3,6,7-tetrahydro-
1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)butyl]amino]hexyl]amino]carbonyl]phen
oxy]carbonyl]-10-methylacridinium-2-yl]methyl]amino]carbonyl]phenyl]-
2,3,6,7,12,13,16,17-octahydro-, inner salt, salt with trifluoroacetic acid
(1:1:1) (9CI) (CA INDEX NAME)

CM 1

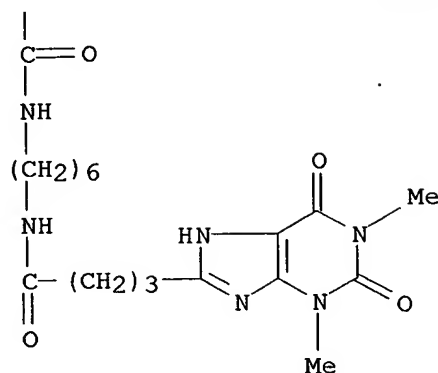
CRN 216669-94-2

CMF C75 H77 N10 O10

PAGE 1-A



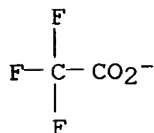
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



IT 216668-60-9P 216873-96-0P 216874-06-5P

216874-10-1P 216973-01-2P

RL: ARU (Analytical role, unclassified); IMF (Industrial manufacture);

ANST (Analytical study); PREP (Preparation)

(prepn. of **chemiluminescent** energy transfer conjugates for
labels in binding assays)

RN 216668-60-9 HCAPLUS

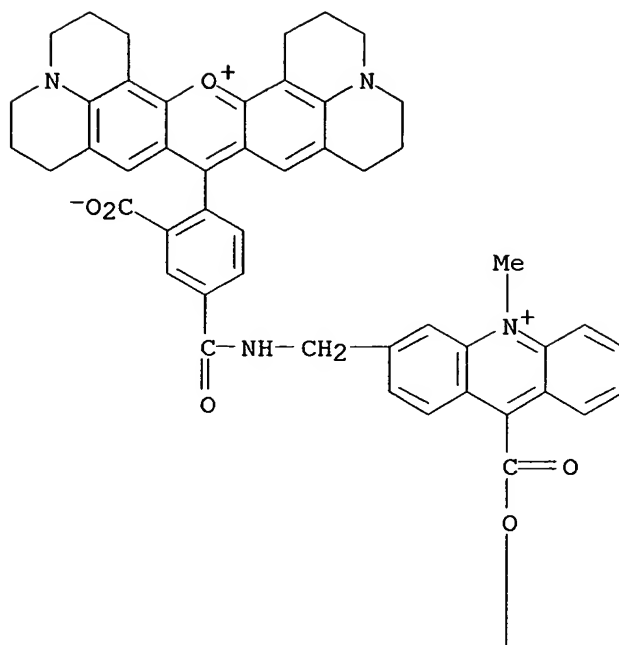
CN 1H,5H,11H,15H-Xantheno[2,3,4-ij:5,6,7-i'j']diquinolizin-18-ium,
9-[2-carboxy-4-[[[9-[[4-[[2-carboxyethyl)amino]carbonyl]-2,6-
dimethylphenoxy]carbonyl]-10-methylacridinium-3-
yl)methyl]amino]carbonyl]phenyl]-2,3,6,7,12,13,16,17-octahydro-, inner
salt, salt with trifluoroacetic acid (1:1:1) (9CI) (CA INDEX NAME)

CM 1

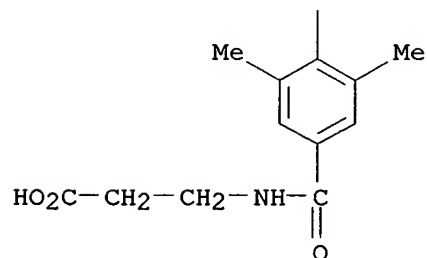
CRN 216668-59-6

CMF C61 H56 N5 O9

PAGE 1-A



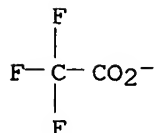
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 216873-96-0 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy) carbonyl]-2-[[[3(or

4)-carboxy-4(or 3)-(2,3,6,7,12,13,16,17-octahydro-1H,5H,11H,15H-xantheno[2,3,4-ij:5,6,7-i',j']diquinolizin-18-ium-9-yl)benzoyl]amino]methyl]-10-methyl-, inner salt, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

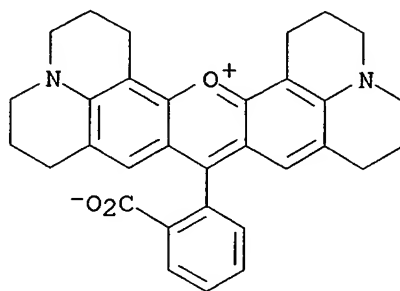
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CRN 216873-95-9

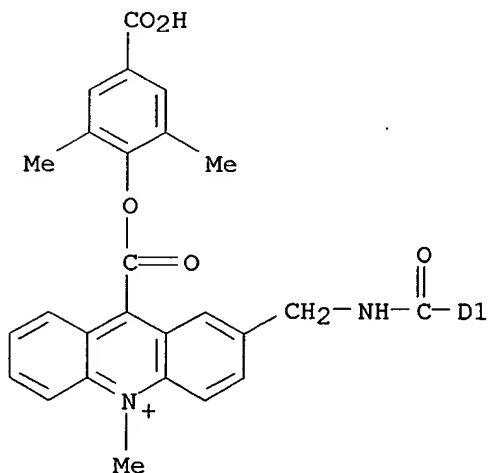
CMF C58 H51 N4 O8

CCI IDS

PAGE 1-A



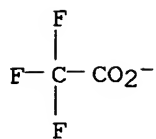
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2

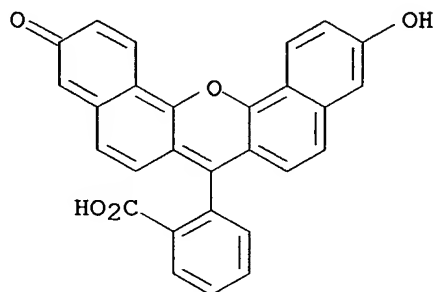


RN 216874-06-5 HCAPLUS
 CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-2-[[[3(or 4)-carboxy-4(or 3)-(11-hydroxy-3-oxo-3H-dibenzo[c,h]xanthen-7-yl)benzoyl]amino]methyl]-10-methyl-, salt with trifluoroacetic acid (1:1)
 (9CI) (CA INDEX NAME)

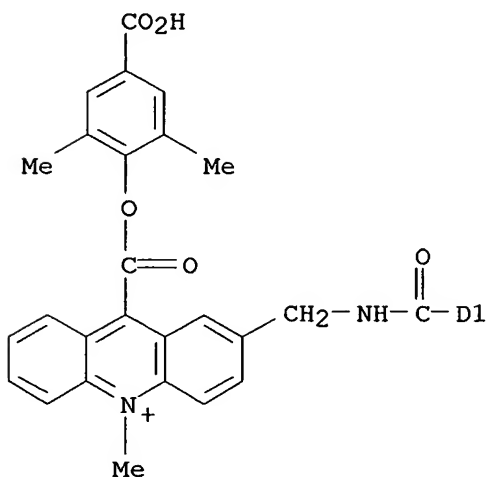
CM 1

CRN 216874-05-4
 CMF C54 H37 N2 O10
 CCI IDS

PAGE 1-A



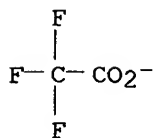
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 216874-10-1 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-3-
 [[[[2(or 4)-(2,3,6,7,12,13,16,17-octahydro-1H,5H,11H,15H-xantheno[2,3,4-
 ij:5,6,7-i'j']diquinolizin-18-ium-9-yl)-5(or 3)-
 sulfophenyl]sulfonyl]amino]methyl]-, inner salt, salt with trifluoroacetic
 acid (1:1) (9CI) (CA INDEX NAME)

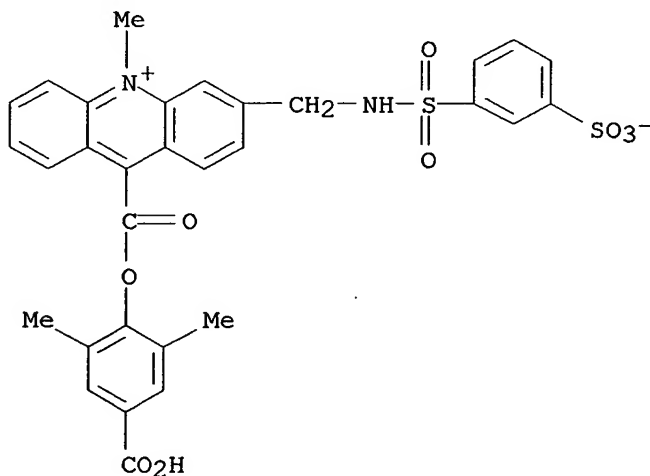
CM 1

CRN 216874-09-8

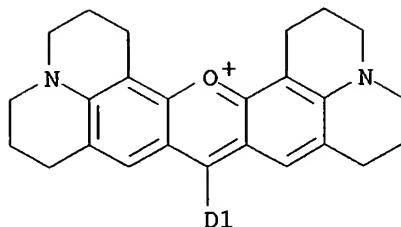
CMF C56 H51 N4 O10 S2

CCI IDS

PAGE 1-A



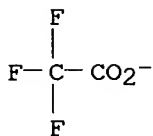
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 216973-01-2 HCAPLUS

CN Acridinium, 9-[[4-[[[(2-carboxyethyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-3-[[[6-[[[2(or 4)-(2,3,6,7,12,13,16,17-octahydro-1H,5H,11H,15H-xantheno[2,3,4-ij:5,6,7-i'j']diquinolizin-18-ium-9-yl)-5-sulfophenyl]sulfonyl]amino]-1-oxohexyl]amino]methyl]-, inner salt, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

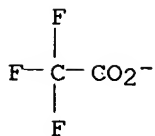
CRN 216973-00-1

CMF C65 H67 N6 O12 S2

CCI IDS

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CMF C2 F3 O2



CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy) carbonyl]-10-methyl-2-

[[[[[2(or 4)-(2,3,6,7,12,13,16,17-octahydro-1H,5H,11H,15H-xantheno[2,3,4-
ij:5,6,7-i'j']diquinolizin-18-ium-9-yl)-5-sulfophenyl]sulfonyl]amino]methy
l]-, inner salt, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX
NAME)

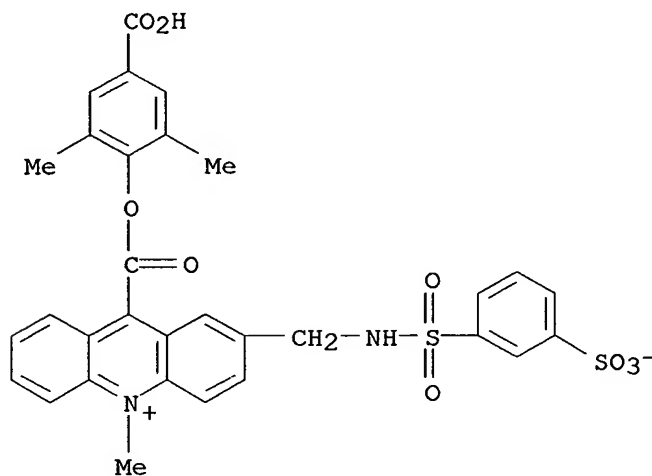
CM 1

CRN 216873-81-3

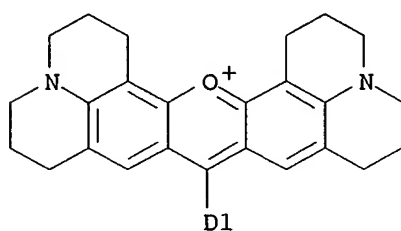
CMF C56 H51 N4 O10 S2

CCI IDS

PAGE 1-A



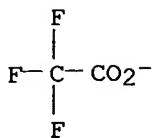
PAGE 2-A



CM 2

CRN 14477-72-6

CMF C2 F3 O2



L10 ANSWER 8 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:699810 HCAPLUS

DOCUMENT NUMBER: 130:20048

TITLE: Detection of reaction intermediates by flow injection electrospray ionization mass spectrometry: reaction of **chemiluminescent** N-sulfonylacridinium-9-carboxamides with hydrogen peroxide

AUTHOR(S): Adamczyk, Maciej; Fishpaugh, Jeffrey R.; Gebler, John C.; Mattingly, Phillip G.; Shreder, Kevin

CORPORATE SOURCE: Diagnostics Division, Division Organic Chemistry (9-NM), Abbott Laboratories, Abbott Park, IL, 60064, USA

SOURCE: European Mass Spectrometry (1998), 4(2), 121-125
CODEN: EMSPFW; ISSN: 1356-1049

PUBLISHER: IM Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

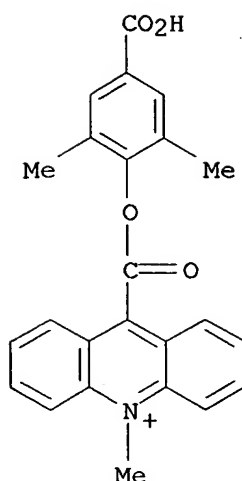
AB Flow injection electrospray mass spectrometry was used to detect the intermediates and products formed during the reaction of **chemiluminescent** acridinium salts under the conditions necessary for light emission. A stream of aq. alk. hydrogen peroxide was mixed with an aq. soln. of N-sulfonylacridinium-9-carboxamide salt immediately prior to entering the ESI-MS interface. The resulting neg.-ion mass spectra corresponded to the expected 9-hydroperoxide adduct, the acridone end product normally seen in the **chemiluminescent** reaction, and unreacted acridinium salt, with no indication of the postulated spirodioxetanone intermediate or competing pseudobase.

IT 148794-24-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(detection of reaction intermediates by flow injection electrospray ionization mass spectrometry for **chemiluminescent** reaction of N-sulfonylacridinium-9-carboxamides with hydrogen peroxide)

RN 148794-24-5 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:13680 HCAPLUS

DOCUMENT NUMBER: 128:72655

TITLE: **Chemiluminescent** group-containing carbodiimide compound

INVENTOR(S): Suzuki, Osamu; Masuda, Gen; Shiohata, Namiko; Matsumoto, Kazuko

PATENT ASSIGNEE(S): Nisshinbo Industries, Inc., Japan

SOURCE: Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| EP 812823 | A1 | 19971217 | EP 1997-303431 | 19970520 |
| EP 812823 | B1 | 20010816 | | |
| R: DE, FR, GB | | | | |
| JP 09328620 | A2 | 19971222 | JP 1996-149553 | 19960611 |
| US 5912344 | A | 19990615 | US 1997-858127 | 19970519 |
| PRIORITY APPLN. INFO.: | | | JP 1996-149553 | A 19960611 |

OTHER SOURCE(S): MARPAT 128:72655

AB Using the **chemiluminescent** group-contg. (acridinium ester group-contg.) carbodiimide compd. or its quaternary ammonium salt as the label in the nucleic acid detection method or immunoassay, labeling can be made efficiently for a short time, a nucleic acid derived from nature can be labeled, and highly sensitive assay is enabled. Synthesis of quaternary salt of **chemiluminescent** group-contg. carbodiimide compd. is described.

IT 200507-90-0

RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)

(**chemiluminescent** group-contg. carbodiimide compd.)

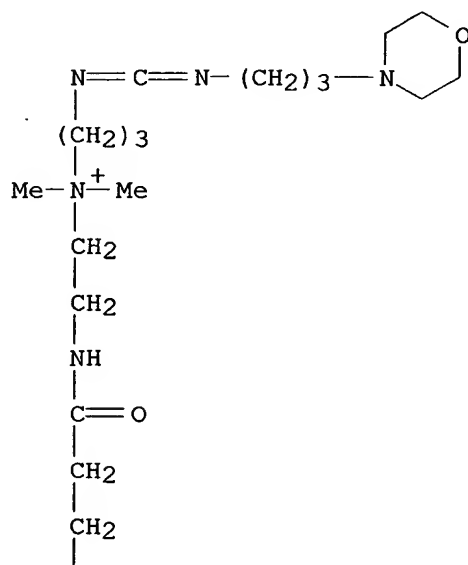
RN 200507-90-0 HCAPLUS
CN Acridinium, 9-[[4-[7,7-dimethyl-16-(4-morpholinyl)-3-oxo-4,11,13-triaza-7-azoniahexadeca-11,12-dien-1-yl]phenoxy]carbonyl]-10-methyl-, bromide fluorosulfate (9CI) (CA INDEX NAME)

CM 1

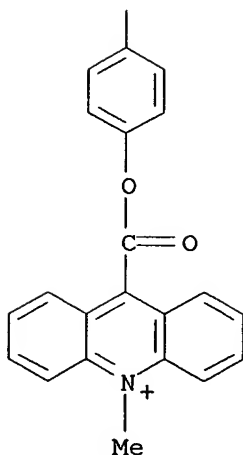
CRN 200507-89-7

CMF C39 H50 N6 O4

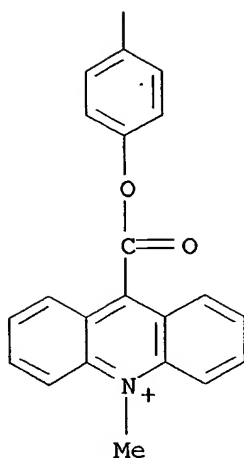
PAGE 1-A



PAGE 2-A



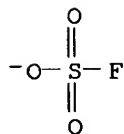
PAGE 2-A



CM 2

CRN 15181-47-2

CMF F O3 S



IT 200508-04-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (chemiluminescent group-contg. carbodiimide compd.)

RN 200508-04-9 HCAPLUS

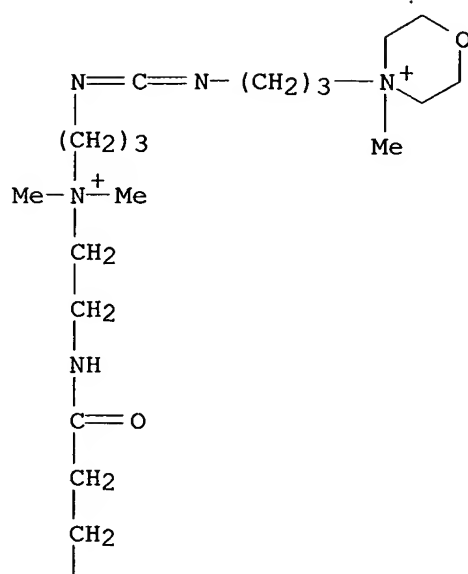
CN Acridinium, 9-[[4-[7,7-dimethyl-16-(4-methylmorpholinium-4-yl)-3-oxo-4,11,13-triaza-7-azoniahexadeca-11,12-dien-1-yl]phenoxy]carbonyl]-10-methyl-, bromide fluorosulfate, salt with 4-methylbenzenesulfonic acid (1:1:1:1) (9CI) (CA INDEX NAME)

CM 1

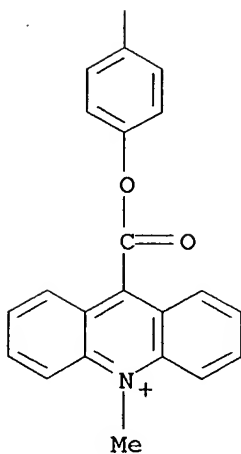
CRN 200508-03-8

CMF C40 H53 N6 O4

PAGE 1-A



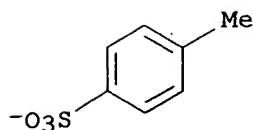
PAGE 2-A



CM 2

CRN 16722-51-3

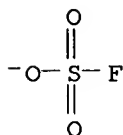
CMF C7 H7 O3 S



CM 3

CRN 15181-47-2

CMF F O3 S



L10 ANSWER 10 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1997:609620 HCAPLUS
 DOCUMENT NUMBER: 127:259776
 TITLE: Nucleophilic polysubstituted aryl acridinium ester
 conjugates and their syntheses
 INVENTOR(S): Law, Say-jong
 PATENT ASSIGNEE(S): Chiron Diagnostics Corp., USA
 SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 871,601.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 5663074 | A | 19970902 | US 1993-32947 | 19930317 |
| US 5241070 | A | 19930831 | US 1992-871601 | 19920417 |
| US 5538901 | A | 19960723 | US 1994-292946 | 19940818 |
| US 6080591 | A | 20000627 | US 1997-920372 | 19970829 |
| PRIORITY APPLN. INFO.: | | | US 1988-249620 | B1 19880926 |
| | | | US 1992-871601 | A2 19920417 |
| | | | US 1993-32085 | B1 19930317 |
| | | | US 1993-32947 | A1 19930317 |

OTHER SOURCE(S): MARPAT 127:259776

AB This invention is directed to novel nucleophilic polysubstituted aryl acridinium conjugates and methods for their prepn. The novel nucleophilic polysubstituted aryl acridinium conjugates are useful as luminescent labels in biol. assays, esp. binding assays, including novel assays for the detn. of vitamin B12, folate, cortisol, estradiol, and thromboxane B2.

IT 196080-94-1P 196080-96-3P 196080-98-5P
 196081-00-2P 196081-01-3P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (nucleophilic polysubstituted aryl acridinium ester conjugates prepn.)

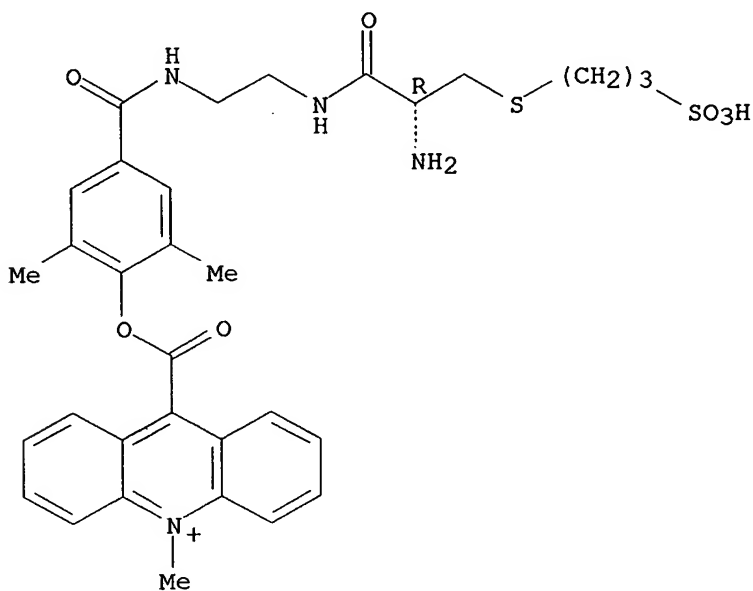
as labels for binding assays)

RN 196080-94-1 HCAPLUS

CN Acridinium, 9-[[4-[[[2-[[2-amino-1-oxo-3-[(3-sulfopropyl)thio]propyl]amino]ethyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

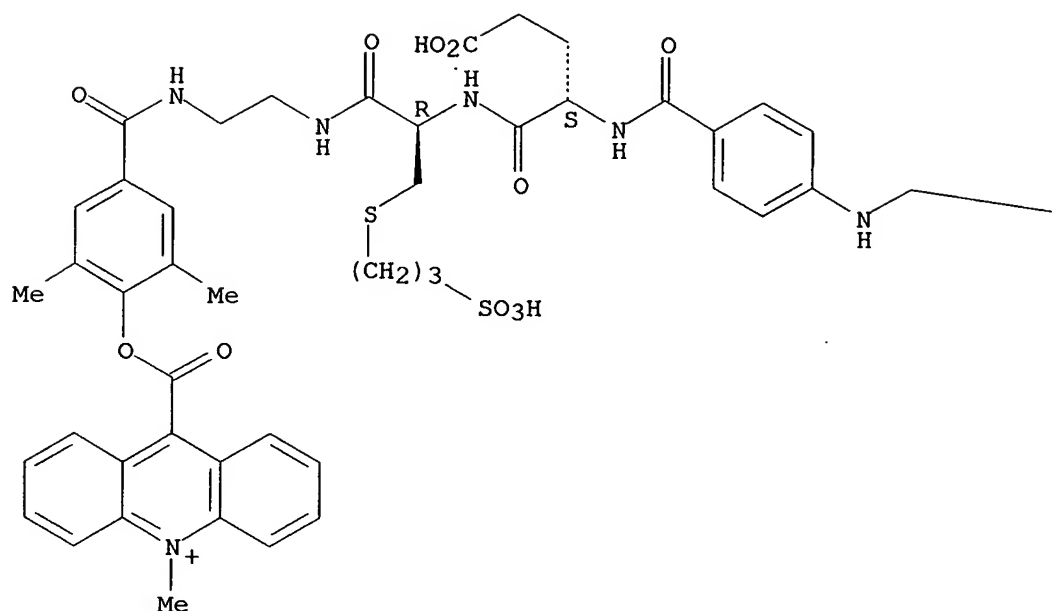
● Br⁻

RN 196080-96-3 HCAPLUS

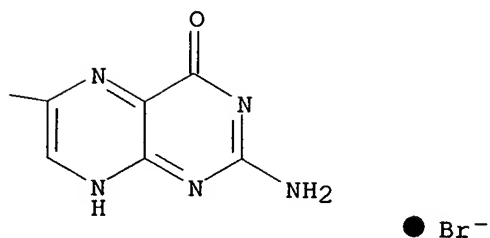
CN L-Cysteinamide, N-[4-[[[2-amino-1,4-dihydro-4-oxo-6-pteridiny]methyl]amino]benzoyl]-L-.alpha.-glutamyl-N-[2-[[[3,5-dimethyl-4-[[[10-methylacridinium-9-yl]carbonyl]oxy]benzoyl]amino]ethyl]-S-(3-sulfopropyl)-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



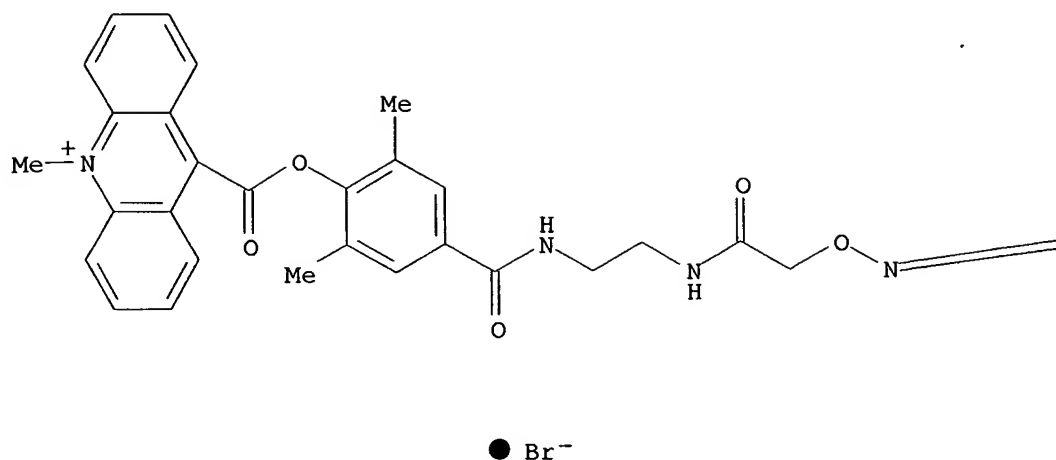
RN 196080-98-5 HCAPLUS

CN Acridinium, 9-[[2,6-dimethyl-4-[[[2-[[[[[(11.beta.)-11,17,21-trihydroxy-20-oxo-19-norpregn-4-en-3-ylidene]amino]oxy]acetyl]amino]ethyl]amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

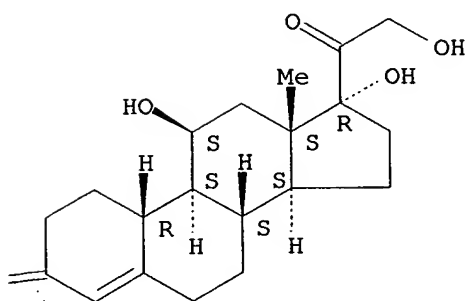
Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A



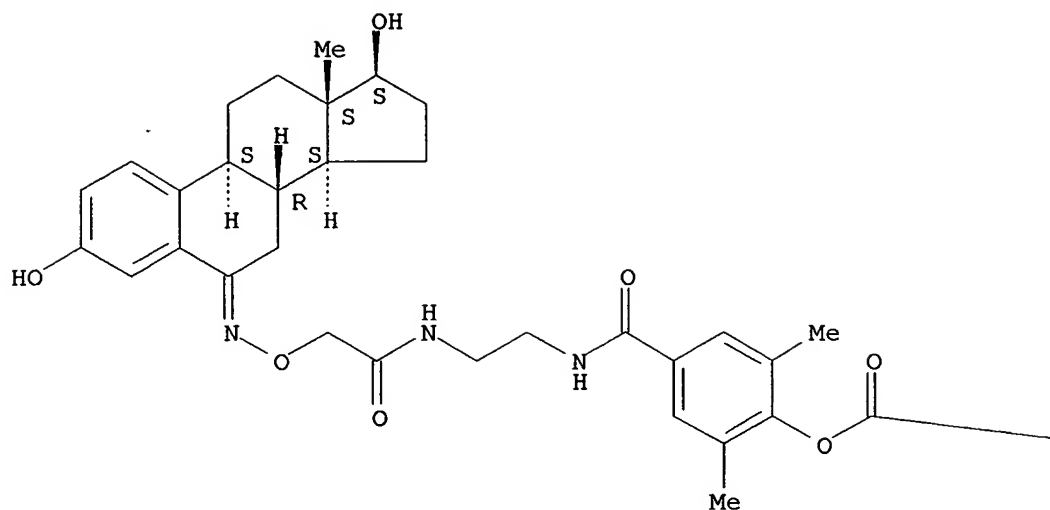
PAGE 1-B



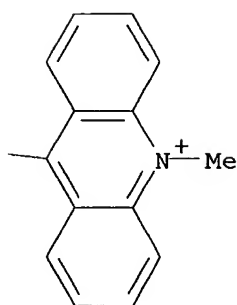
RN 196081-00-2 HCAPLUS
 CN Acridinium, 9-[[4-[[[2-[[[(17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-6-ylidene]amino]oxy]acetyl]amino]ethyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

PAGE 1-A



PAGE 1-B

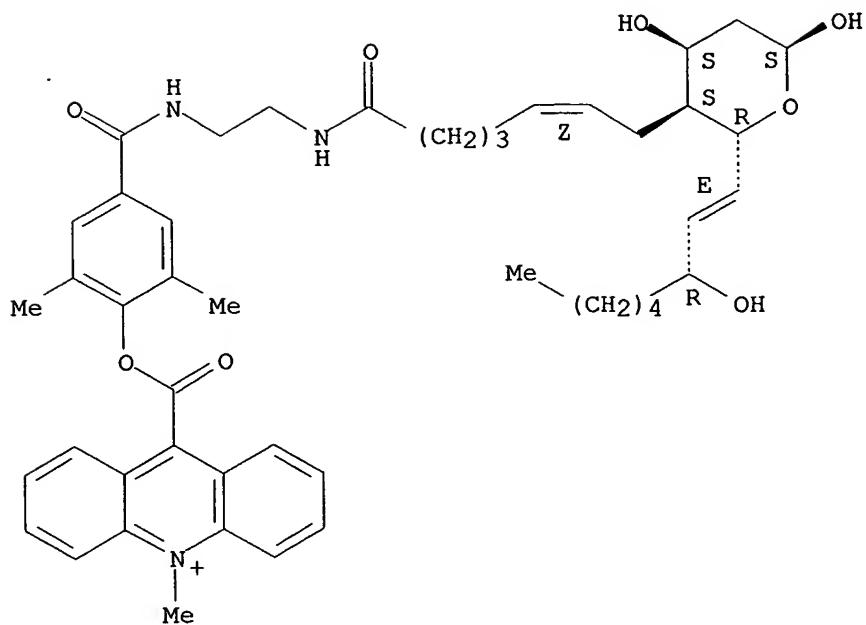
● Br⁻

RN 196081-01-3 HCAPLUS

CN Acridinium, 9-[[2,6-dimethyl-4-[[[2-[[1-oxo-7-[tetrahydro-4,6-dihydroxy-2-(3-hydroxy-1-octenyl)-2H-pyran-3-yl]-5-heptenyl]amino]ethyl]amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide, [2R-[2.alpha.(1E,3R*),3.beta.(Z),4.beta.,6.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 2-A

● Br⁻

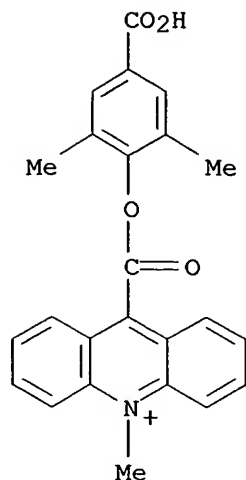
IT 123655-39-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(nucleophilic polysubstituted aryl acridinium ester conjugates prepn.
as labels for binding assays)

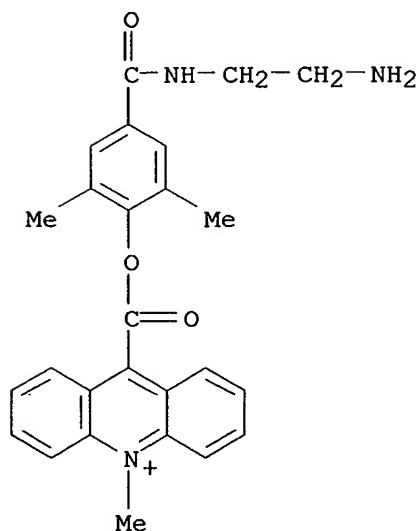
RN 123655-39-0 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-,
bromide (9CI) (CA INDEX NAME)



● Br⁻

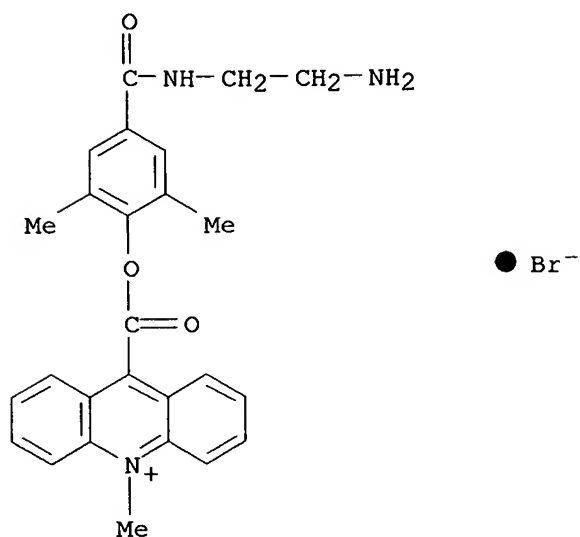
IT **123655-38-9DP**, reaction product with vitamin B12 monocarboxylates
123655-38-9P 130772-56-4P 196080-97-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (nucleophilic polysubstituted aryl acridinium ester conjugates prepn.
 as labels for binding assays)
 RN 123655-38-9 HCAPLUS
 CN Acridinium, 9-[[4-[[2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 123655-38-9 HCAPLUS
 CN Acridinium, 9-[[4-[[2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

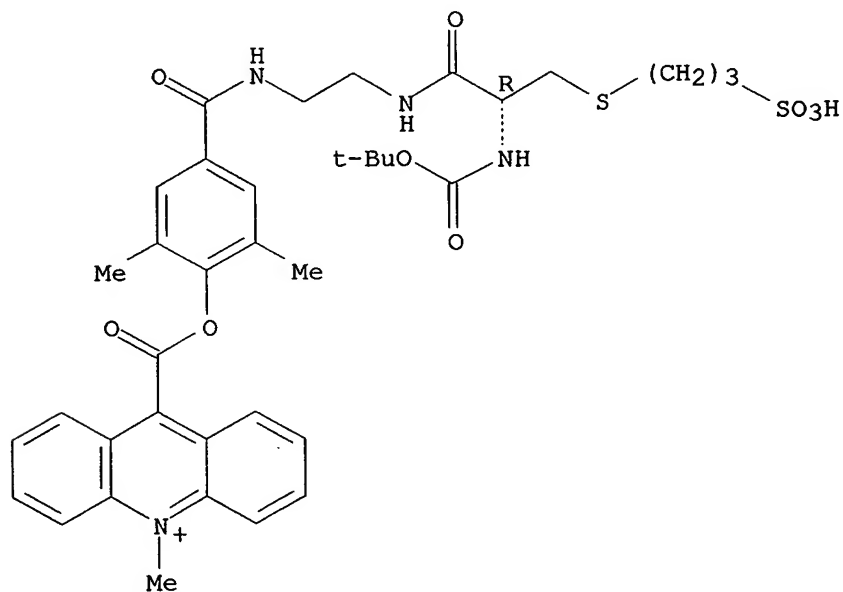


RN 130772-56-4 HCAPLUS

CN Acridinium, 9-[[4-[11,11-dimethyl-1,6,9-trioxo-7-[[[3-sulfopropyl)thio]methyl]-10-oxa-2,5,8-triazadodec-1-yl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

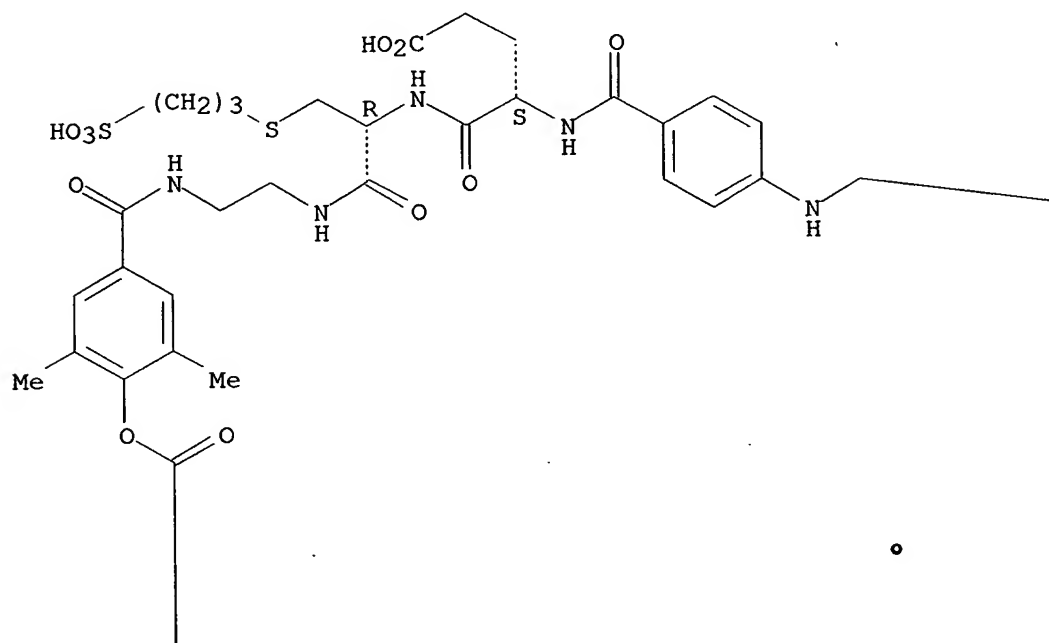
● Br⁻

RN 196080-97-4 HCAPLUS

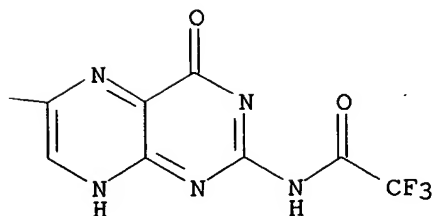
CN L-Cysteinamide, N-[4-[[[1,4-dihydro-4-oxo-2-[(trifluoroacetyl)amino]-6-pteridiny]methyl]amino]benzoyl]-L-.alpha.-glutamyl-N-[2-[[3,5-dimethyl-4-[[[(10-methylacridinium-9-yl)carbonyl]oxy]benzoyl]amino]ethyl]-S-(3-sulfopropyl)-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

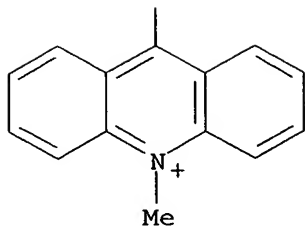
PAGE 1-A



PAGE 1-B



PAGE 2-A

● Br⁻

L10 ANSWER 14 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1997:574406 HCAPLUS
 DOCUMENT NUMBER: 127:187871
 TITLE: Functionalized hydrophilic acridinium esters
 INVENTOR(S): Law, Say-Jong; Sotiriou-Leventis, Chariklia; Natrajan, Anand; Jiang, Qingping; Connolly, Peter B.; Kilroy, John P.; McCudden, Constance R.; Tirrell, Stephen M.
 PATENT ASSIGNEE(S): Chiron Diagnostics Corp., USA
 SOURCE: U.S., 28 pp., Cont.-in-part of U.S. 5,449,556.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 5656426 | A | 19970812 | US 1994-225165 | 19940408 |
| JP 09025422 | A2 | 19970128 | JP 1996-179488 | 19890731 |
| US 5227489 | A | 19930713 | US 1992-826186 | 19920122 |
| US 5449556 | A | 19950912 | US 1993-32231 | 19930317 |
| US 5595875 | A | 19970121 | US 1994-325845 | 19941019 |
| CA 2186463 | AA | 19951019 | CA 1995-2186463 | 19950406 |
| WO 9527702 | A1 | 19951019 | WO 1995-IB244 | 19950406 |
| W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA | | | | |
| RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9520816 | A1 | 19951030 | AU 1995-20816 | 19950406 |
| AU 703436 | B2 | 19990325 | | |
| EP 754178 | A1 | 19970122 | EP 1995-913298 | 19950406 |
| EP 754178 | B1 | 20030115 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI | | | | |
| BR 9507307 | A | 19970902 | BR 1995-7307 | 19950406 |
| JP 10503169 | T2 | 19980324 | JP 1995-526216 | 19950406 |
| EP 982298 | A1 | 20000301 | EP 1999-203889 | 19950406 |

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI
 AT 231130 E 20030215 AT 1995-913298 19950406
 US 5656500 A 19970812 US 1995-440427 19950512
 PRIORITY APPLN. INFO.:
 US 1988-226639 B1 19880801
 US 1992-826186 A3 19920122
 US 1993-32231 A2 19930317
 JP 1989-199178 A3 19890731
 US 1993-32321 A3 19930317
 US 1994-225165 A 19940408
 US 1994-325845 A1 19941019
 EP 1995-913298 A3 19950406
 WO 1995-IB244 W 19950406

OTHER SOURCE(S): MARPAT 127:187871

AB Novel acridinium esters are disclosed that are useful, either alone or when incorporated into liposomes, as **chemiluminescent** agents in binding assays (e.g., immunoassays and gene probe assays) with improved sensitivity. In addn., the synthesis of these esters and their use in assays for detecting an analyte are described. In particular, assays for testosterone and the Rubella virus are disclosed.

IT **173406-73-0P 173406-74-1P 173406-75-2P**

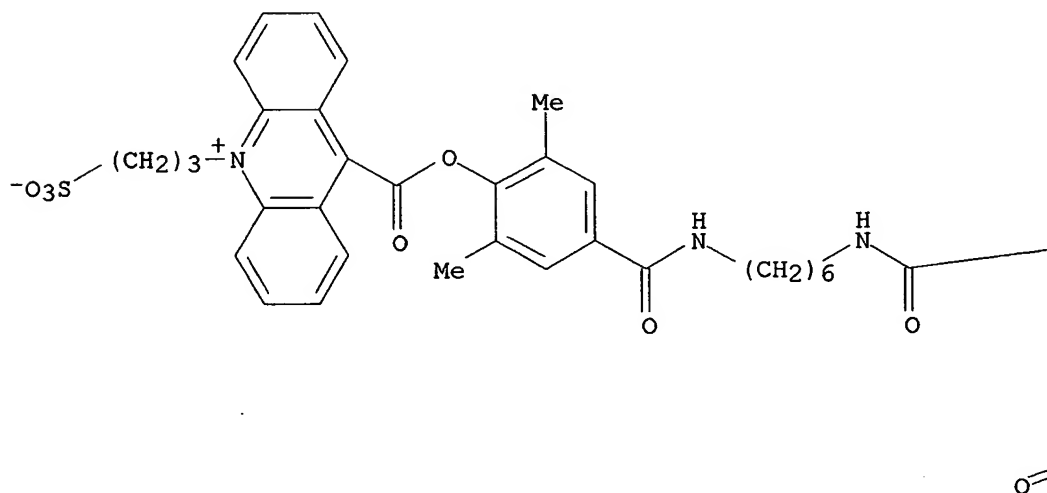
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (functionalized hydrophilic acridinium esters prepn. for binding assays)

RN 173406-73-0 HCAPLUS

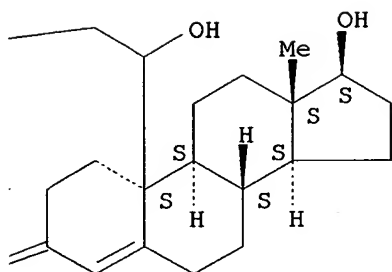
CN Acridinium, 9-[[4-[[[6-[[3-hydroxy-3-[(17.beta.)-17-hydroxy-3-oxoestr-4-en-10-yl]-1-oxopropyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

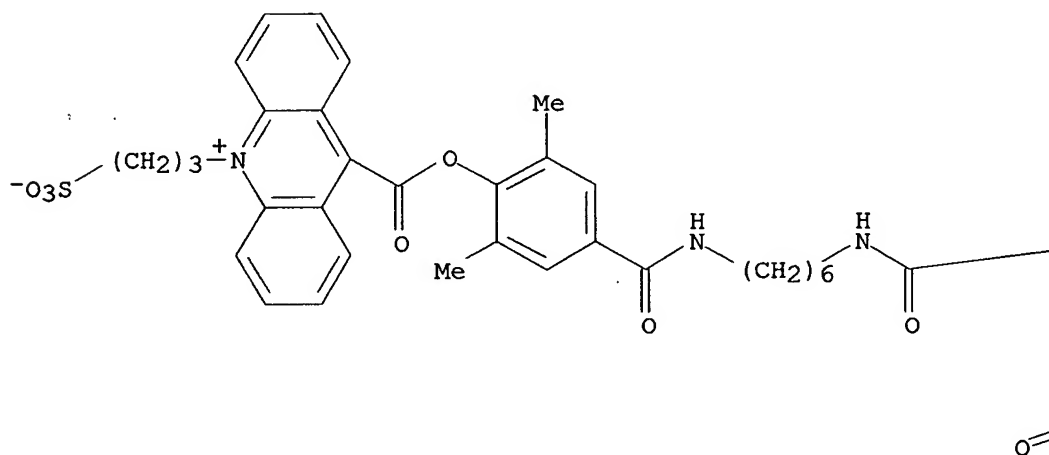


RN 173406-74-1 HCAPLUS

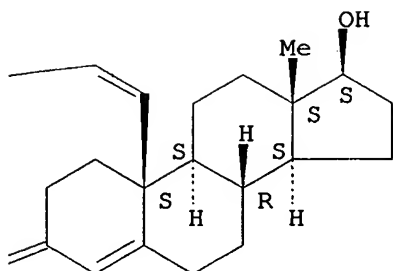
CN Acridinium, 9-[[4-[[[6-[[3-[(17.beta.)-17-hydroxy-3-oxoestr-4-en-10-yl]-1-oxo-2-propenyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 1-B

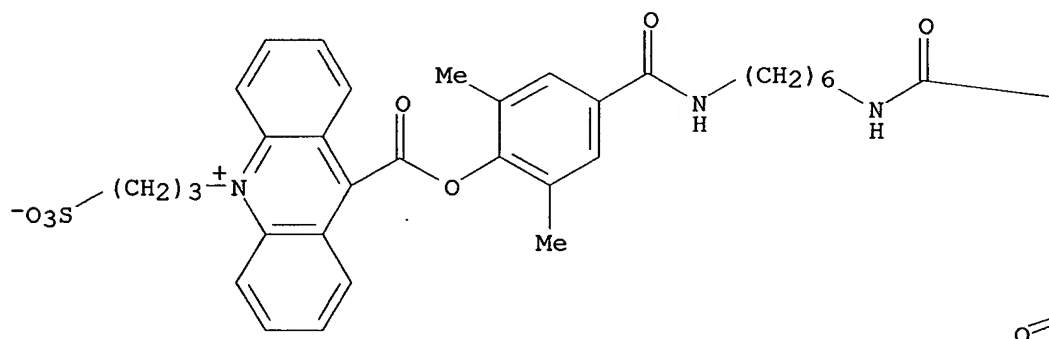


RN 173406-75-2 HCAPLUS

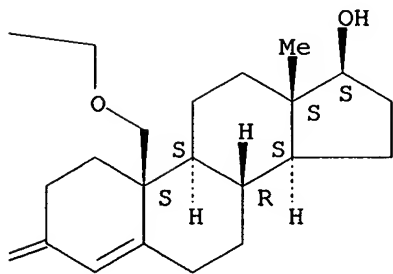
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Absolute stereochemistry.

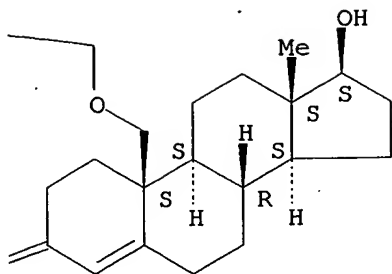
PAGE 1-A



PAGE 1-B



PAGE 1-B



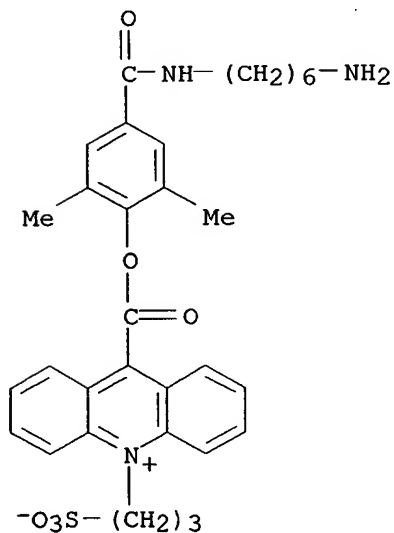
IT 194357-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(functionalized hydrophilic acridinium esters prepn. for binding assays)

RN 194357-76-1 HCAPLUS

CN Acridinium, 9-[[4-[[[(6-aminohexyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)



L10 ANSWER 31 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:72257 HCAPLUS

DOCUMENT NUMBER: 126:85614

TITLE: Nucleic acid target or other analyte determination using adduct protection assay including labeled analyte-binding probe and ligand which alters signal of unbound probe

INVENTOR(S): Becker, Michael; Nelson, Norman C.

PATENT ASSIGNEE(S): Gen-Probe Incorporated, USA

SOURCE: Eur. Pat. Appl., 37 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 747706 | A1 | 19961211 | EP 1996-108880 | 19960603 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE | | | | |
| US 5731148 | A | 19980324 | US 1995-478221 | 19950607 |
| CA 2222556 | AA | 19961219 | CA 1996-2222556 | 19960523 |
| WO 9641197 | A1 | 19961219 | WO 1996-US7776 | 19960523 |
| W: AU, CA, JP, KR | | | | |
| AU 9660244 | A1 | 19961230 | AU 1996-60244 | 19960523 |
| AU 703605 | B2 | 19990325 | | |
| JP 2002515118 | T2 | 20020521 | JP 1997-500745 | 19960523 |

PRIORITY APPLN. INFO.:
 US 1995-478221 A 19950607
 WO 1996-US7776 W 19960523

OTHER SOURCE(S): MARPAT 126:85614

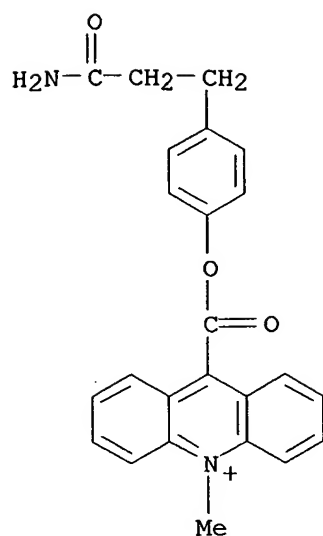
AB The present invention features an adduct protection assay involving the use of a labeled binding partner and a signal altering ligand. The signal altering ligand can preferentially alter the ability of label which is not part of a binding partner:analyte complex to produce a detectable signal, compared to its ability to alter signal produced from label which is part of a binding partner:analyte complex. The presence or amt. of analyte can be detd. by detecting the signal produced from unaltered label. The adduct protection assay is very versatile. For example, alteration of signal can be carried out under a wide range of conditions (e.g., pH, temp., and ionic strength), and both label alteration and signal triggering can be carried out at essentially const. temp. to achieve a high degree of sensitivity.

IT 185102-40-3 185102-41-4 185102-42-5
 185102-44-7 185606-16-0

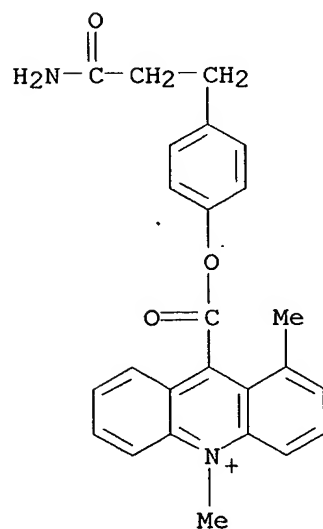
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (signal-altering ligand; nucleic acid target or other analyte detn.
 using adduct protection assay including labeled analyte-binding probe
 and ligand which alters signal of unbound probes)

RN 185102-40-3 HCAPLUS

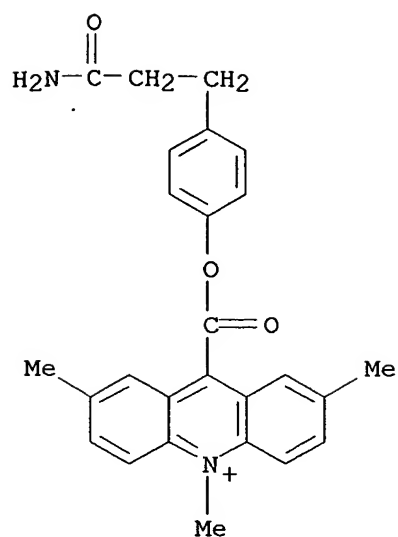
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 (CA INDEX NAME)



RN 185102-41-4 HCAPLUS
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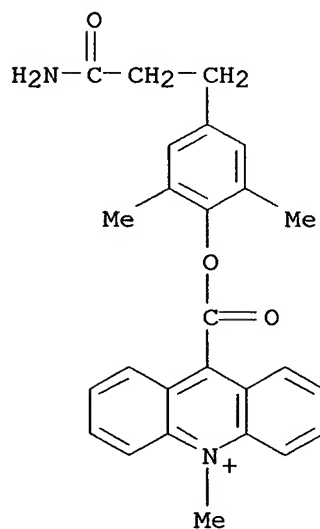


RN 185102-42-5 HCAPLUS
 CN Acridinium, 9-[[4-(3-amino-3-oxopropyl)phenoxy]carbonyl]-2,7,10-trimethyl-
 (9CI) (CA INDEX NAME)



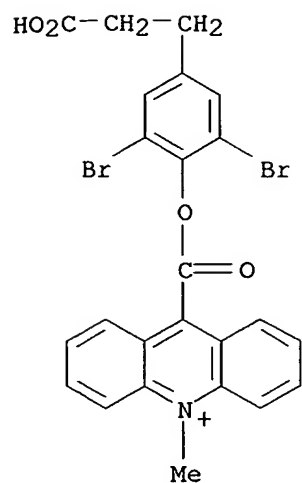
RN 185102-44-7 HCAPLUS

CN Acridinium, 9-[[4-(3-amino-3-oxopropyl)-2,6-dimethylphenoxy]carbonyl]-10-methyl- (9CI) (CA INDEX NAME)



RN 185606-16-0 HCAPLUS

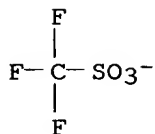
CN Acridinium, 9-[[4-(3-amino-3-oxo-1-propenyl)-2-methoxyphenoxy]carbonyl]-10-methyl- (9CI) (CA INDEX NAME)



CM 2

CRN 37181-39-8

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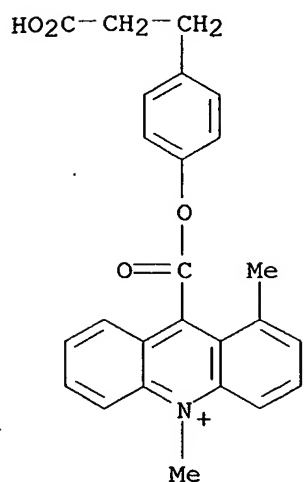
RN 177332-67-1 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-1,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-66-0

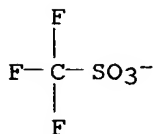
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CM 2

CRN 37181-39-8

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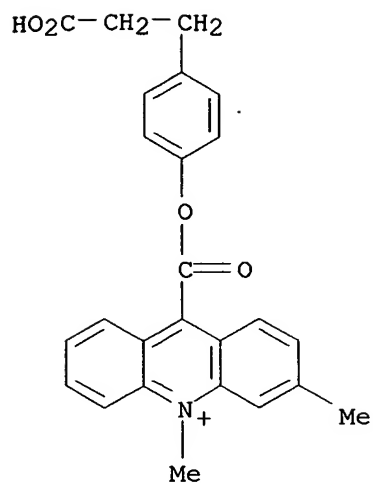
RN 177332-69-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-3,10-dimethyl-, salt
with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-68-2

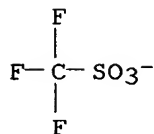
CMF C25 H22 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



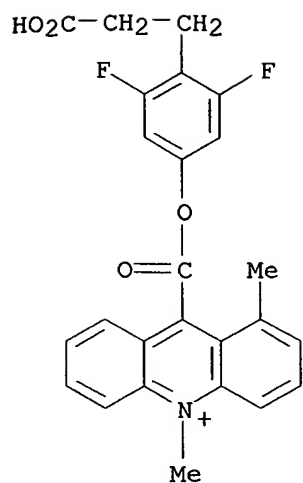
RN 177332-71-7 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-1,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

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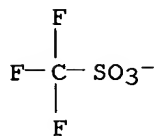
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CM 2

CRN 37181-39-8

CMF C F3 O3 S



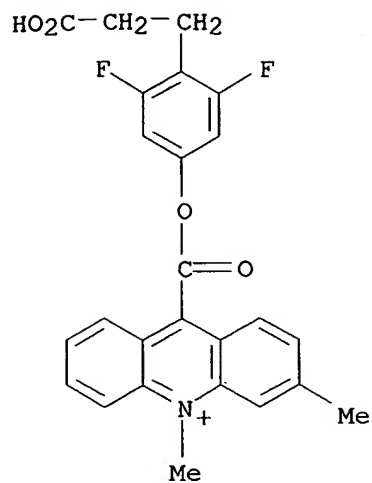
RN 177332-73-9 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-3,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-72-8

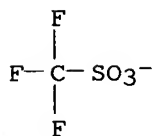
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CM 2

CRN 37181-39-8

CMF C F3 O3 S



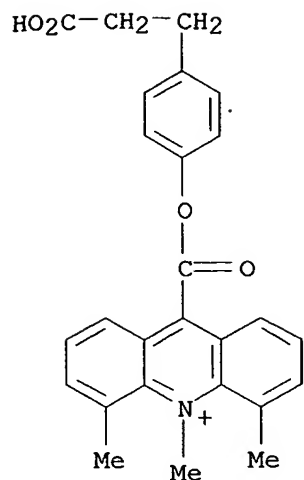
RN 177409-05-1 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-4,5,10-trimethyl-,
salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177409-04-0

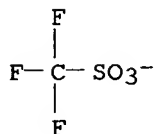
CMF C26 H24 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



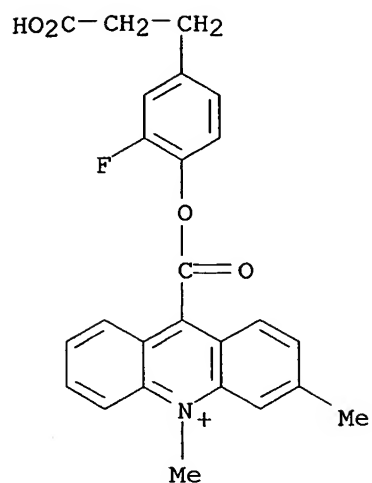
RN 177409-07-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2-fluorophenoxy]carbonyl]-3,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177409-06-2

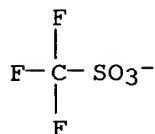
CMF C25 H21 F N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



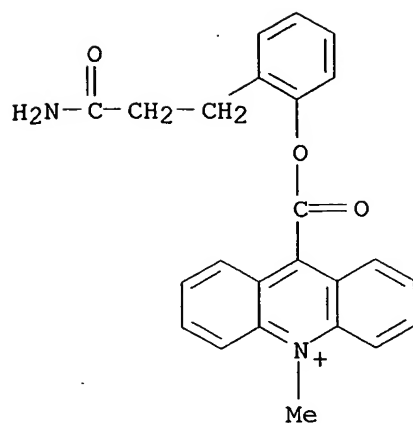
RN 177409-09-5 HCAPLUS

CN Acridinium, 9-[[2-(3-amino-3-oxopropyl)phenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177409-08-4

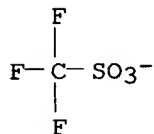
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CM 2

CRN 37181-39-8

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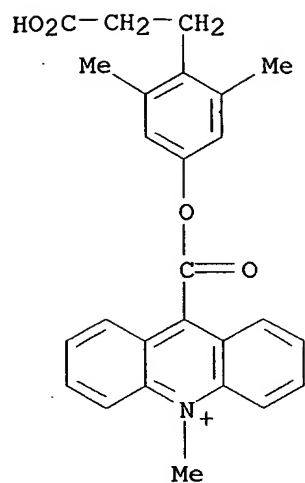
RN 177409-11-9 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-dimethylphenoxy]carbonyl]-10-methyl-
 , salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177409-10-8

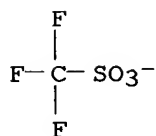
CMF C26 H24 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



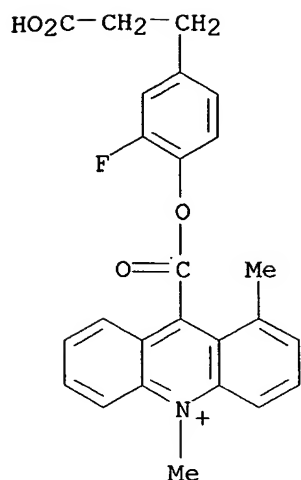
RN 177409-13-1 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2-fluorophenoxy]carbonyl]-1,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177409-12-0

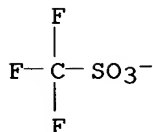
CMF C25 H21 F N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



L10 ANSWER 15 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:332777 HCAPLUS

DOCUMENT NUMBER: 125:2414

TITLE: Simultaneous detection of multiple nucleic acid targets in a homogeneous format

AUTHOR(S): Nelson, Norman C.; Cheikh, Azzouz Ben; Matsuda, Eiji; Becker, Michael M.

CORPORATE SOURCE: Gen-Probe Inc., San Diego, CA, 92121, USA

SOURCE: Biochemistry (1996), 35(25), 8429-8438

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The acridinium ester 4-(2-succinimidylloxycarbonyl)phenyl-10-methylacridinium 9-carboxylate trifluoromethane sulfonate (AE), which reacts rapidly with alk. hydrogen peroxide to produce light, has been used as a detection label in a no. of assay procedures, including nucleic acid probe-based systems. A no. of derivs. of this AE were synthesized and their **chemiluminescent** properties characterized. These derivs. display significant differences in the kinetics of the **chemiluminescence** reaction as well as optimal pH for light prodn. These differences allow two or more derivs. to be simultaneously detected and quantitated in a single reaction vessel. Several of these derivs.

have been covalently linked to nucleic acid probe mols. and have been further characterized in regard to **chemiluminescence** properties as well as hydrolysis of the ester bond in both single- and double-stranded conformations. On the basis of these properties, homogeneous assay formats utilizing DNA probes labeled with various AE derivs. were developed. Simultaneous detection and quantitation of Chlamydia trachomatis and Neisseria gonorrhoeae, the gag and pol regions of HIV, and wild-type and mutant HIV sequences was achieved with high sensitivity and discrimination.

IT 177332-30-8 177332-32-0 177332-34-2
177332-36-4 177332-39-7 177332-43-3
177332-47-7 177332-49-9 177332-51-3

RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)

(**chemiluminescent** acridinium ester labels for the simultaneous detection and quantification of multiple nucleic acid sequences by hybridization)

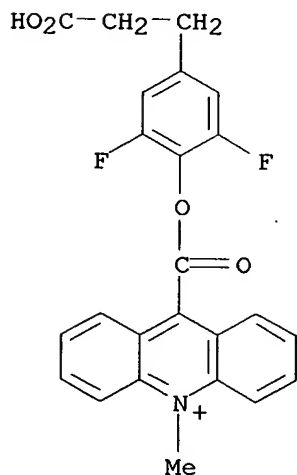
RN 177332-30-8 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2,6-difluorophenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-29-5

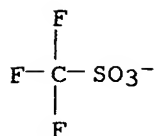
CMF C24 H18 F2 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



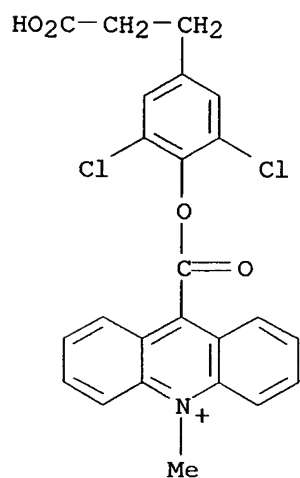
RN 177332-32-0 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2,6-dichlorophenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-31-9

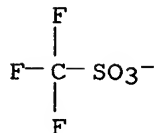
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CM 2

CRN 37181-39-8

CMF C F3 O3 S



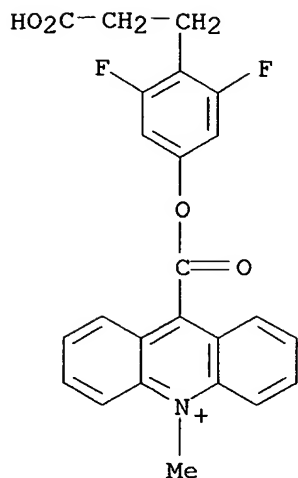
RN 177332-34-2 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-33-1

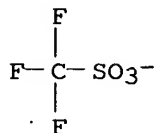
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CM 2

CRN 37181-39-8

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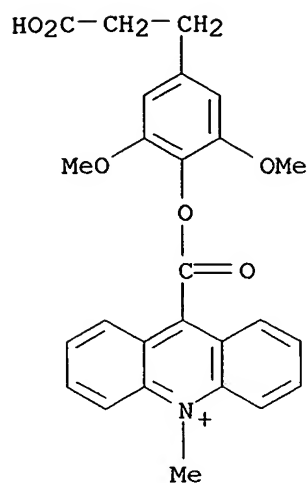
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CN Acridinium, 9-[[4-(2-carboxyethyl)-2,6-dimethoxyphenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-35-3

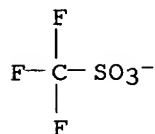
CMF C26 H24 N O6



CM 2

CRN 37181-39-8

CMF C F3 O3 S



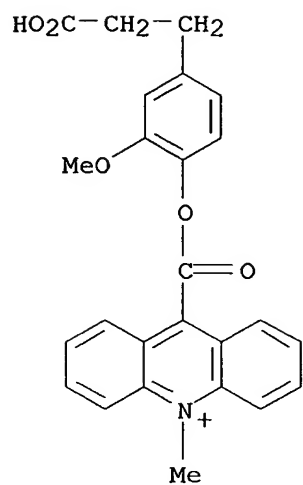
RN 177332-39-7 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2-methoxyphenoxy]carbonyl]-10-methyl-,
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CM 1

CRN 177332-38-6

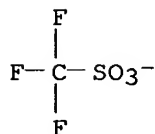
CMF C25 H22 N O5



CM 2

CRN 37181-39-8

CMF C F3 O3 S



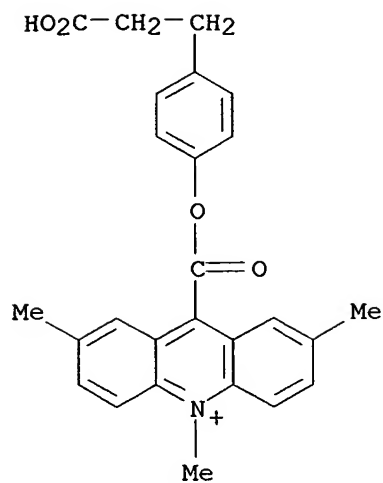
RN 177332-43-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-2,7,10-trimethyl-,
salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-42-2

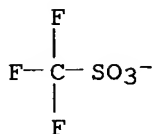
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CM 2

CRN 37181-39-8

CMF C F3 O3 S



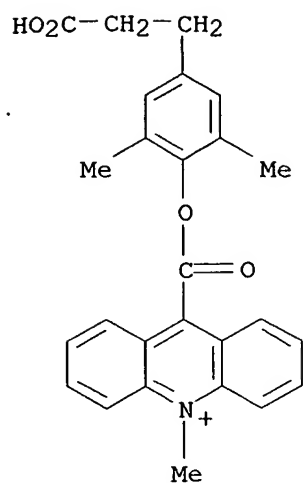
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CN Acridinium, 9-[[4-(2-carboxyethyl)-2,6-dimethylphenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-46-6

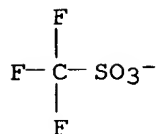
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CM 2

CRN 37181-39-8

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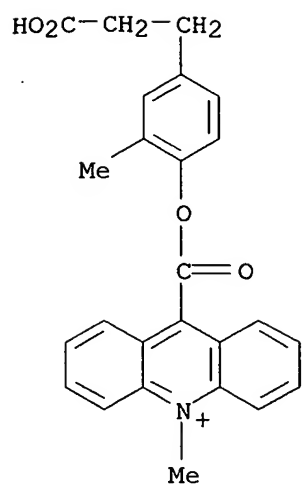
RN 177332-49-9 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2-methylphenoxy]carbonyl]-10-methyl-,
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CM 1

CRN 177332-48-8

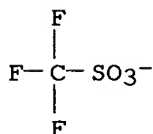
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CM 2

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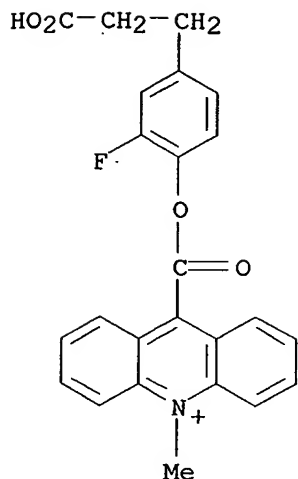
RN 177332-51-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-2-fluorophenoxy]carbonyl]-10-methyl-,
salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-50-2

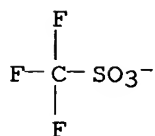
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CM 2

CRN 37181-39-8

CMF C F3 O3 S



IT 177332-61-5P 177332-63-7P 177332-65-9P
 177332-67-1P 177332-69-3P 177332-71-7P
 177332-73-9P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (chemiluminescent acridinium ester labels for the simultaneous detection and quantification of multiple nucleic acid sequences by hybridization)

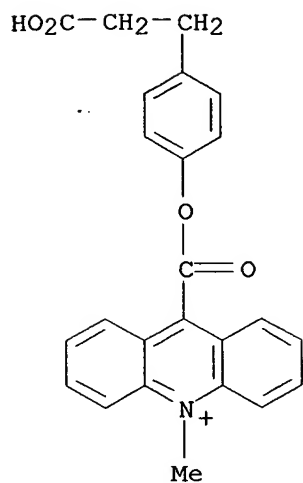
RN 177332-61-5 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-60-4

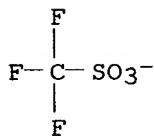
CMF C24 H20 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



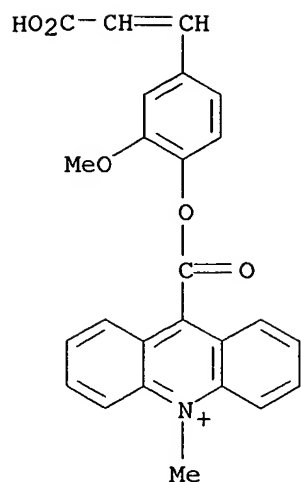
RN 177332-63-7 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethenyl)-2-methoxyphenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-62-6

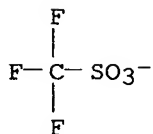
CMF C25 H20 N O5



CM 2

CRN 37181-39-8

CMF C F3 O3 S



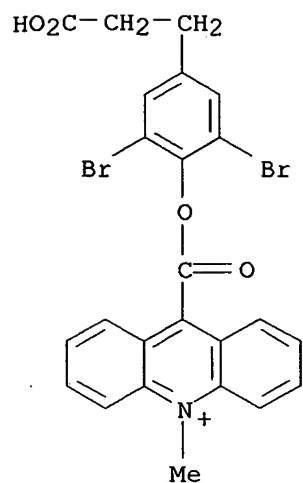
RN 177332-65-9 HCAPLUS

CN Acridinium, 9-[[2,6-dibromo-4-(2-carboxyethyl)phenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-64-8

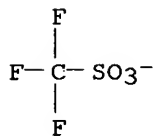
CMF C24 H18 Br2 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



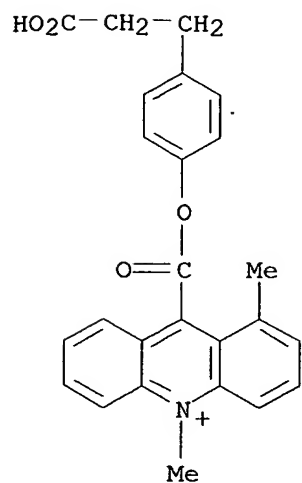
RN 177332-67-1 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-1,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-66-0

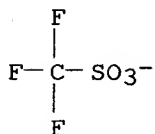
CMF C25 H22 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



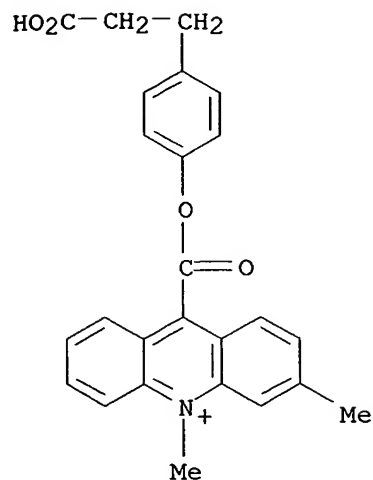
RN 177332-69-3 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)phenoxy]carbonyl]-3,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-68-2

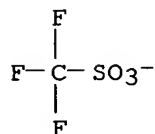
CMF C25 H22 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



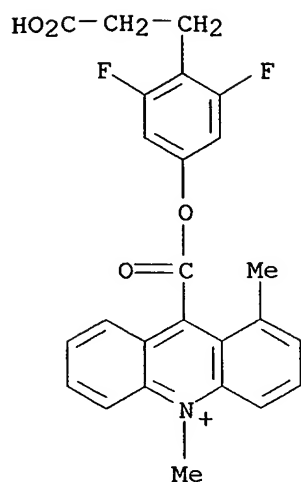
RN 177332-71-7 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-1,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-70-6

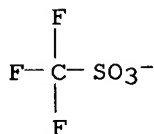
CMF C25 H20 F2 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



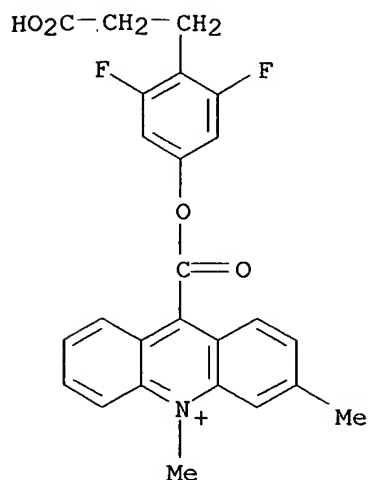
RN 177332-73-9 HCAPLUS

CN Acridinium, 9-[[4-(2-carboxyethyl)-3,5-difluorophenoxy]carbonyl]-3,10-dimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 177332-72-8

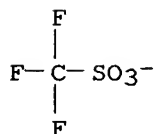
CMF C25 H20 F2 N O4



CM 2

CRN 37181-39-8

CMF C F3 O3 S



L10 ANSWER 16 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1995:996620 HCAPLUS
 DOCUMENT NUMBER: 124:140396
 TITLE: Novel functionalized hydrophilic acridinium esters
 INVENTOR(S): Law, Say-jong; Sotiriou-Leventis, Chaiklia; Natrajan, Anand; Jiang, Qingping; Connolly, Peter B.; Kilroy, John P.; Mccudden, Constance R.; Tirrell, Stephen M.
 PATENT ASSIGNEE(S): Ciba Corning Diagnostics Corp., USA
 SOURCE: PCT Int. Appl., 71 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 9527702 | A1 | 19951019 | WO 1995-IB244 | 19950406 |
| W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA | | | | |
| RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, | | | | |

LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
SN, TD, TG

| | | | | |
|------------|----|----------|----------------|----------|
| US 5656426 | A | 19970812 | US 1994-225165 | 19940408 |
| AU 9520816 | A1 | 19951030 | AU 1995-20816 | 19950406 |
| AU 703436 | B2 | 19990325 | | |
| EP 754178 | A1 | 19970122 | EP 1995-913298 | 19950406 |
| EP 754178 | B1 | 20030115 | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI

| | | | | |
|-------------|----|----------|----------------|----------|
| BR 9507307 | A | 19970902 | BR 1995-7307 | 19950406 |
| JP 10503169 | T2 | 19980324 | JP 1995-526216 | 19950406 |
| AT 231130 | E | 20030215 | AT 1995-913298 | 19950406 |

PRIORITY APPLN. INFO.:

| | | |
|----------------|----|----------|
| US 1994-225165 | A1 | 19940408 |
| US 1988-226639 | B1 | 19880801 |
| US 1992-826186 | A3 | 19920122 |
| US 1993-32231 | A2 | 19930317 |
| WO 1995-IB244 | W | 19950406 |

OTHER SOURCE(S): MARPAT 124:140396

AB Novel acridinium esters that are useful, either alone or when incorporated into liposomes, as **chemiluminescent** agents in binding assays (e.g., immunoassays and gene probe assays) with improved sensitivity are disclosed. In addn., the synthesis of these esters and their use in assays for detecting an analyte is described. In particular, assays for testosterone and the rubella virus are disclosed. In example, synthesis of acridinium ester for immunoassay of testosterone, anti-Rubella virus IgG, and TSH was described.

IT **173406-73-0P 173406-74-1P 173406-75-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

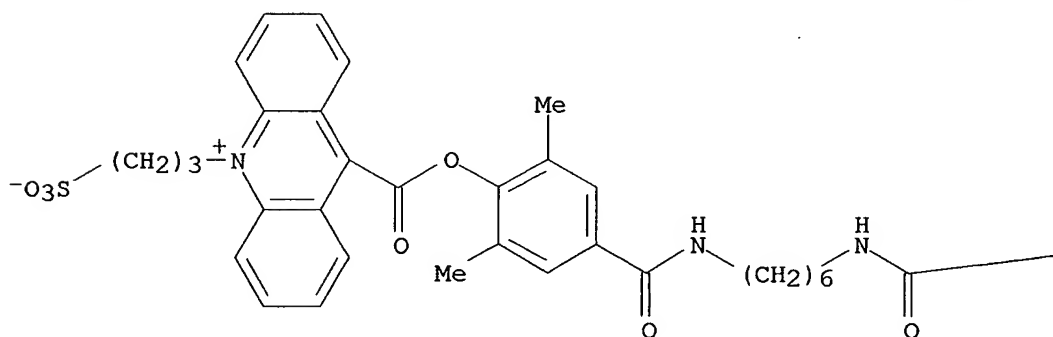
(prepn. of conjugates of functionalized hydrophilic acridinium esters for immunoassay or as gene probe)

RN 173406-73-0 HCAPLUS

CN Acridinium, 9-[[4-[[[6-[[3-hydroxy-3-[(17.beta.)-17-hydroxy-3-oxoestr-4-en-10-yl]-1-oxopropyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

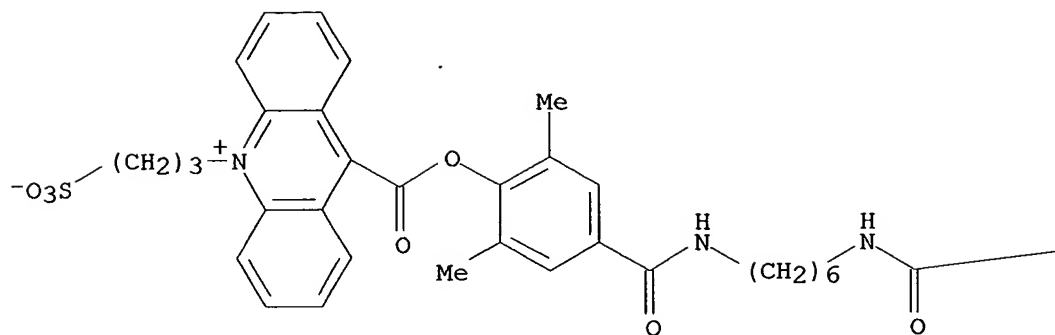
Absolute stereochemistry.

PAGE 1-A

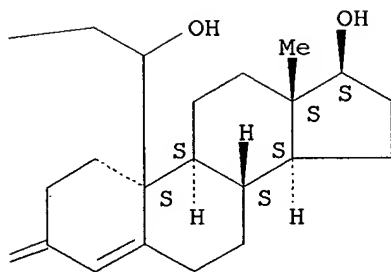


O=

PAGE 1-A



PAGE 1-B



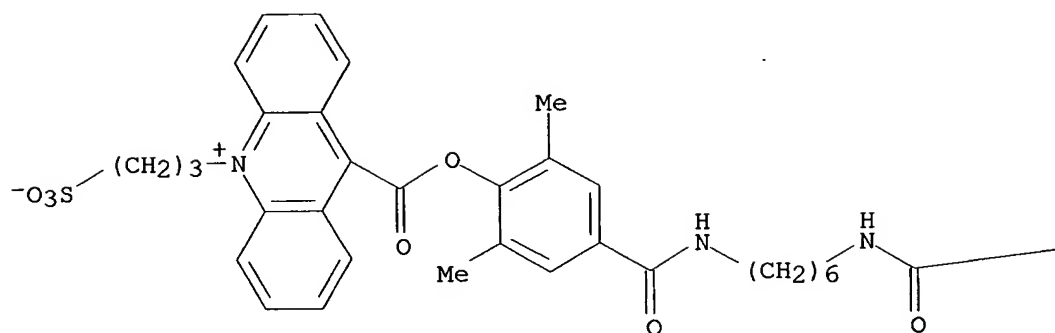
RN 173406-74-1 HCAPLUS

CN Acridinium, 9-[[4-[[[6-[[3-[(17.beta.)-17-hydroxy-3-oxoestr-4-en-10-yl]-1-oxo-2-propenyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

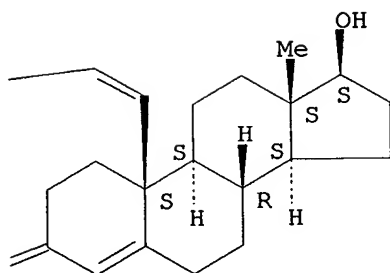
Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A



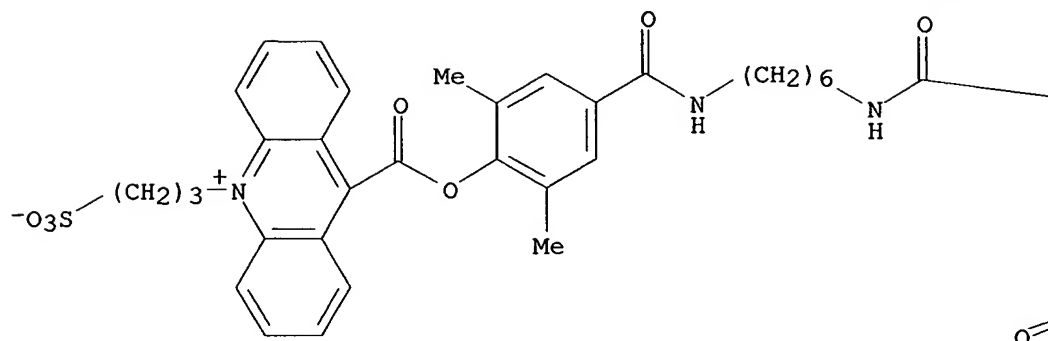
PAGE 1-B



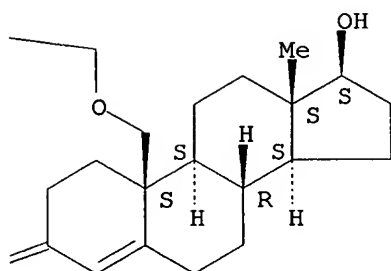
RN 173406-75-2 HCAPLUS
 CN Acridinium, 9-[[4-[[[6-[[[(17.beta.)-17-hydroxy-3-oxoandrost-4-en-19-yl]oxy]acetyl]amino]hexyl]amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L10 ANSWER 17 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:362383 HCAPLUS

DOCUMENT NUMBER: 122:133003

TITLE: Preparation of N-alkylacridancarboxyl derivatives useful for **chemiluminescent** assays.

INVENTOR(S): Akhavan-Tafti, Hashem; Desilva, Renuka; Sugioka, Katsuaki

PATENT ASSIGNEE(S): Lumigen, Inc., USA

SOURCE: Eur. Pat. Appl., 40 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

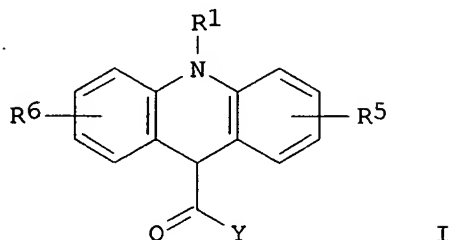
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 12

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 625510 | A2 | 19941123 | EP 1994-107632 | 19940517 |
| EP 625510 | A3 | 19970305 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| US 5491072 | A | 19960213 | US 1993-61810 | 19930517 |
| CA 2123235 | AA | 19941118 | CA 1994-2123235 | 19940510 |
| AU 9463025 | A1 | 19941201 | AU 1994-63025 | 19940512 |

AU 666814 B2 19960222
 WO 9426927 A1 19941124 WO 1994-US5437 19940516
 W: JP
 JP 08500125 T2 19960109 JP 1994-525766 19940516
 JP 3231777 B2 20011126
 PRIORITY APPLN. INFO.: US 1993-61810 A 19930517
 WO 1994-US5437 W 19940516
 OTHER SOURCE(S): MARPAT 122:133003
 GI



AB The title compds. (I; R1 = alkyl, heteroalkyl, aralkyl; R2, R6 = H, noninterfering substituents ; Y = leaving group), which produce light from the reaction of a peroxide and a peroxidase in the presence of an analyte and are thus useful in **chemiluminescent** assays, are prepd. Thus, I (R1 = Me, R5 = R6 = H, Y = OPh) was prepd. from 9-acridinecarboxylic acid in 3 steps.

IT **161006-17-3P 161006-21-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of N-alkylacridancarboxyl derivs. useful for **chemiluminescent** assays)

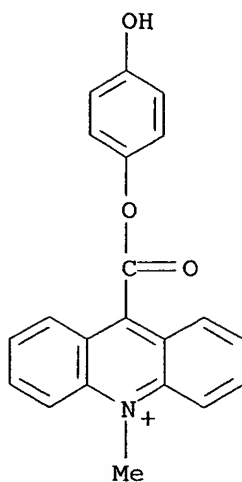
RN 161006-17-3 HCAPLUS

CN Acridinium, 9-[(4-hydroxyphenoxy)carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 161006-16-2

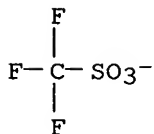
CMF C21 H16 N O3



CM 2

CRN 37181-39-8

CMF C F3 O3 S



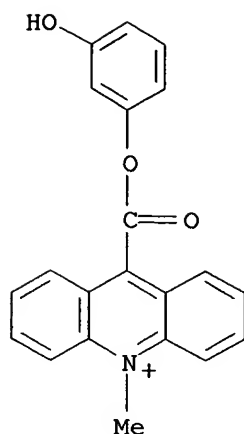
RN 161006-21-9 HCAPLUS

CN Acridinium, 9-[(3-hydroxyphenoxy)carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 161006-20-8

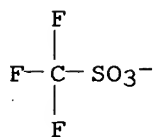
CMF C21 H16 N O3



CM 2

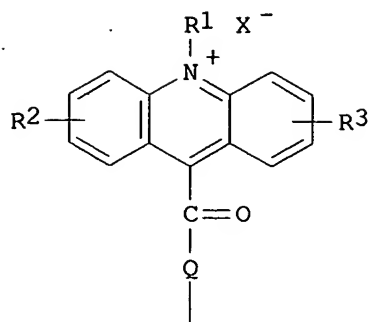
CRN 37181-39-8

CMF C F3 O3 S

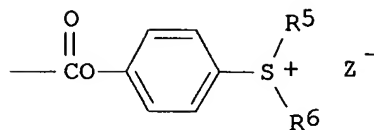


L10 ANSWER 18 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1995:312281 HCAPLUS
 DOCUMENT NUMBER: 122:76051
 TITLE: Acridinium derivative **chemiluminescent**
 indicators
 INVENTOR(S): Odagiri, Takeshi; Kunichika, Makoto
 PATENT ASSIGNEE(S): Sanyo Chemical Ind Ltd, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

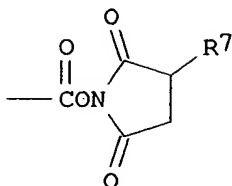
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|------|----------|-----------------|----------|
| JP 06158039 | A2 | 19940607 | JP 1992-335220 | 19921120 |
| PRIORITY APPLN. INFO.: GI | | | JP 1992-335220 | 19921120 |



I



II



III

AB The indicators, suited for use in immunoassay, comprises: 2-5 groups represented by I; and a group selected from II, III, isoindolinedioneoxycarbonyl, p-nitrophenyloxycarbonyl, pentachlorophenyloxycarbonyl, isothiocyanate, isocyanate, and SO₂Cl [R₁ = H, C1-10 alkyl, alkenyl, alkynyl, aryl; R_{2,3} = H, C1-5 alkyl, alkoxy, NH₂, COOH, CN, NO₂, CHO, halo; Q = direct bond, NR₄Y; R₄ = (substituted) C1-10 alkylene, alkenylene, arylene; X⁻ = anion; Y = H, C1-10 alkyl, aryl, alkoxy, aryloxy, COOH, carboalkoxy, carboaryl, carboxamide, NH₂, OH, CN, CHO, morpholino, mercapto, halo; R_{5,6} = (substituted) C1-10 alkyl, alkenyl, alkynyl, aryl].

IT 160453-23-6

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(**chemiluminescent** immunoassay indicators)

RN 160453-23-6 HCAPLUS

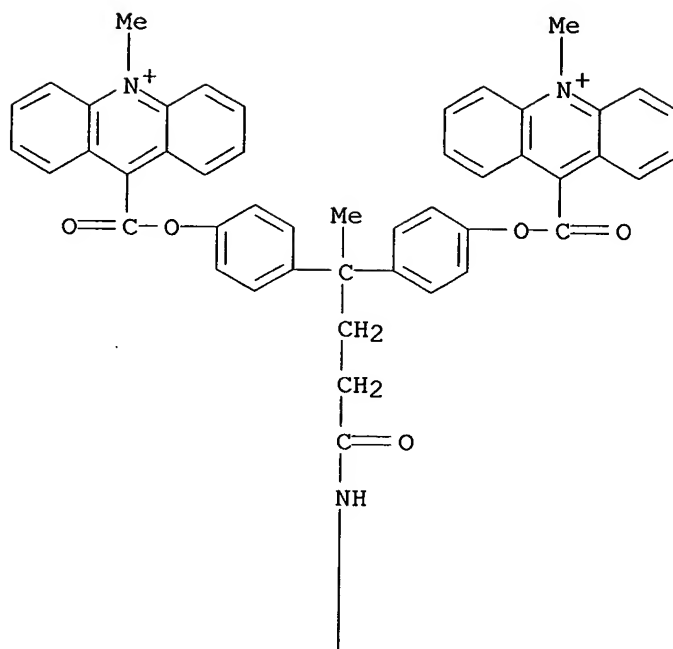
CN Acridinium, 9,9'-[[4-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)phenyl]amino]-1-methyl-4-oxobutylidene]bis(4,1-phenyleneoxycarbonyl)]bis[10-methyl-, bis(fluorosulfate) (9CI) (CA INDEX NAME)

CM 1

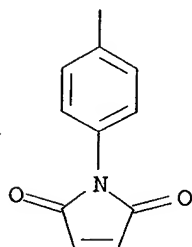
CRN 160453-22-5

CMF C57 H44 N4 O7

PAGE 1-A



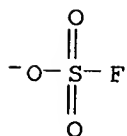
PAGE 2-A



CM 2

CRN 15181-47-2

CMF F O3 S



L10 ANSWER 19 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:277037 HCAPLUS
 DOCUMENT NUMBER: 122:55905
 TITLE: Hydrolytically stable **chemiluminescent** labels and their conjugates, and assays therefrom by adduct formation
 INVENTOR(S): McCapra, Frank
 PATENT ASSIGNEE(S): London Diagnostics, Inc., USA
 SOURCE: U.S., 14 pp. Cont.-in-part of U.S. Ser. No. 140,040, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 7
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 5338847 | A | 19940816 | US 1992-860001 | 19920330 |
| FR 2625565 | A1 | 19890707 | FR 1988-17502 | 19881230 |
| AU 8929270 | A1 | 19890801 | AU 1989-29270 | 19881230 |
| AU 635890 | B2 | 19930408 | | |
| DE 3891212 | T | 19910110 | DE 1988-3891212 | 19881230 |
| JP 03501772 | T2 | 19910418 | JP 1989-501385 | 19881230 |
| JP 3172522 | B2 | 20010604 | | |
| ZA 8900019 | A | 19891129 | ZA 1989-19 | 19890103 |
| GB 2232995 | A1 | 19910102 | GB 1990-14479 | 19900628 |
| GB 2232995 | B2 | 19921014 | | |
| GB 2251942 | A1 | 19920722 | GB 1992-3180 | 19920214 |
| GB 2252161 | A1 | 19920729 | GB 1992-3179 | 19920214 |
| GB 2252162 | A1 | 19920729 | GB 1992-3181 | 19920214 |
| US 5321136 | A | 19940614 | US 1992-860410 | 19920330 |
| PRIORITY APPLN. INFO.: | | | US 1987-140040 | B2 19871231 |
| | | | US 1988-291843 | B2 19881229 |
| | | | US 1989-418956 | B2 19891010 |
| | | | WO 1988-US4719 | A 19881230 |
| | | | GB 1990-14479 | A3 19901230 |

OTHER SOURCE(S): MARPAT 122:55905

AB Described are a class of **chemiluminescent** compds. characterized by the presence an aryl ester, thioester or amide of a carboxylic acid substituted heterocyclic ring that is susceptible to chem. attack (such as by oxidic attack) to dissoc. the heterocyclic ring to a transient compd. The heterocyclic ring is ring carbon-bonded to the carbonyl of the ester, thioester and amide moiety and possesses a heteroatom in an oxidn. state that allows **chemiluminescence** by dissocg. a compd. ("intermediate") that decays to produce **chemiluminescence**, at the carbon bonded to the carbonyl. The aryl ring or ring system is ring carbon-bonded to the oxygen, sulfur or nitrogen of the ester, thioester or amide, as the case may be, and contains at least three substituents on a six-member ring. The substitution on the six-member ring comprises three or more groups acting in concert to sterically and electronically hinder hydrolysis of the ester, thioester or amide linkage. Significant to this invention is the presence of diortho electron donating substitution on the aryl unit in conjunction with meta and/or para substituents that possess a specific level of electron withdrawing capacity. That specific level of electron withdrawing capacity is a .sigma.Rp value greater than 0 and less than 1. In addn., there is the presence of an adduct affixed at the carbon atom of the heterocyclic ring to which the ester, thioester or

amide carbonyl carbon is directly bonded. Also in accordance with the present invention are conjugates of the labeling compn., assay systems utilizing the conjugates, and assay kits incorporating such **chemiluminescent** labels.

IT 126430-78-2P 126430-80-6P 157392-99-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydrolytically stable heterocyclic **chemiluminescent** labels and their conjugates, and assays therefrom by adduct formation)

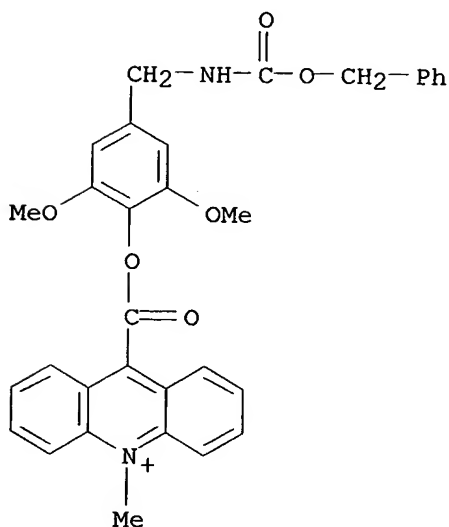
RN 126430-78-2 HCAPLUS

CN Acridinium, 9-[[2,6-dimethoxy-4-[[[(phenylmethoxy)carbonyl]amino]methyl]phenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 126430-77-1

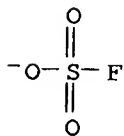
CMF C32 H29 N2 O6



CM 2

CRN 15181-47-2

CMF F O3 S



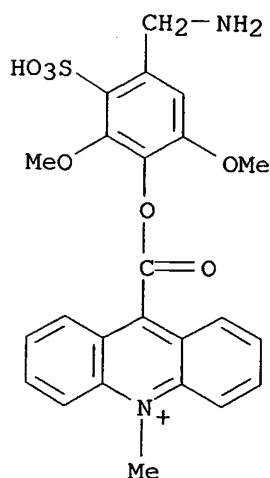
RN 126430-80-6 HCAPLUS

CN Acridinium, 9-[[4-(aminomethyl)-2,6-dimethoxy-3-sulfophenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 126430-79-3

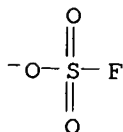
CMF C24 H23 N2 O7 S



CM 2

CRN 15181-47-2

CMF F O3 S



RN 157392-99-9 HCAPLUS

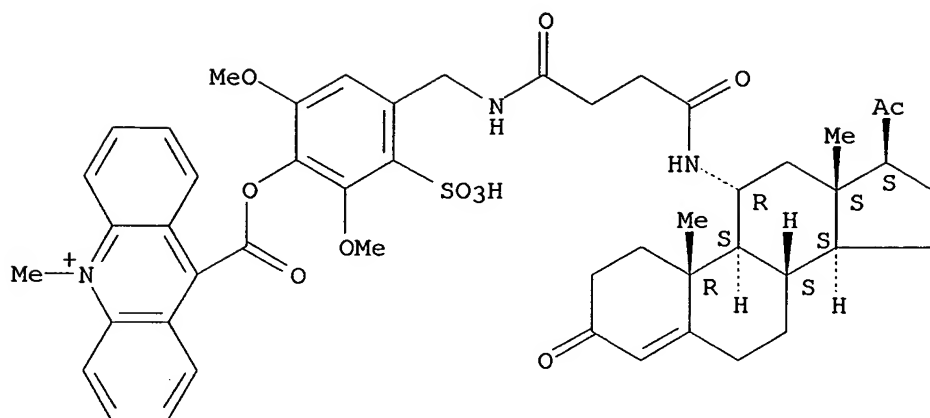
CN Acridinium, 9-[[[2,6-dimethoxy-4-[[[4-[[[11.alpha.)-3,20-dioxopregn-4-en-11-yl]amino]-1,4-dioxobutyl]amino]methyl]-3-sulfophenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157392-98-8

CMF C49 H56 N3 O11 S

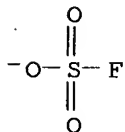
Absolute stereochemistry.



CM 2

CRN 15181-47-2

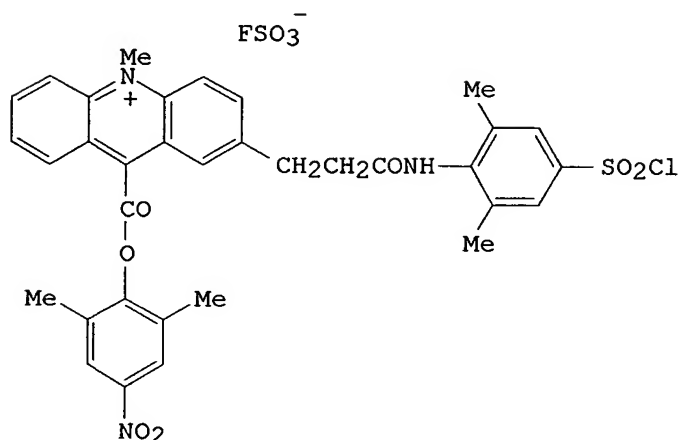
CMF F O3 S



L10 ANSWER 20 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1994:557542 HCAPLUS
 DOCUMENT NUMBER: 121:157542
 TITLE: Preparation of hydrolytically stable
 acridiniumcarboxylates as **chemiluminescent**
 labels and assays therefrom
 INVENTOR(S): McCapra, Frank; Beheshti, Iraj
 PATENT ASSIGNEE(S): London Diagnostics, Inc., USA
 SOURCE: U.S., 33 pp. Cont.-in-part of U.S. Ser. No. 140,040,
 abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 7
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| US 5284951 | A | 19940208 | US 1992-859956 | 19920330 |
| FR 2625565 | A1 | 19890707 | FR 1988-17502 | 19881230 |
| AU 8929270 | A1 | 19890801 | AU 1989-29270 | 19881230 |
| AU 635890 | B2 | 19930408 | | |
| DE 3891212 | T | 19910110 | DE 1988-3891212 | 19881230 |
| JP 03501772 | T2 | 19910418 | JP 1989-501385 | 19881230 |
| JP 3172522 | B2 | 20010604 | | |

| | | | | |
|------------------------|----|----------|-------------------|-------------|
| ZA 8900019 | A | 19891129 | ZA 1989-19 | 19890103 |
| GB 2232995 | A1 | 19910102 | GB 1990-14479 | 19900628 |
| GB 2232995 | B2 | 19921014 | | |
| GB 2251942 | A1 | 19920722 | GB 1992-3180 | 19920214 |
| GB 2252161 | A1 | 19920729 | GB 1992-3179 | 19920214 |
| GB 2252162 | A1 | 19920729 | GB 1992-3181 | 19920214 |
| US 5321136 | A | 19940614 | US 1992-860410 | 19920330 |
| PRIORITY APPLN. INFO.: | | | US 1987-140040 | B2 19871231 |
| | | | US 1988-291843 | B2 19881229 |
| | | | US 1989-418956 | B2 19891010 |
| | | | WO 1988-US4719 | A 19881230 |
| | | | GB 1990-14479 | A3 19901230 |
| OTHER SOURCE(S): | | | MARPAT 121:157542 | |
| GI | | | | |



AB Claimed is a novel **chemiluminescent** compd. comprising an aryl ester, thioester, or amide of a carboxylic acid substituted heterocyclic ring that is susceptible to chem. attack to dissoc. the heterocyclic ring to a transient compd., wherein the heterocyclic ring is ring carbon-bonded to the carbonyl of the ester, thioester or amide moiety and possesses a heteroatom in an oxidn. state that allows **chemiluminescence** by dissocg. a compd. at the carbon bonded to the carbonyl that decays to produce **chemiluminescence**, the aryl is a ring or ring system that is ring carbon-bonded to the oxygen, sulfur, or nitrogen of the ester, thioester, or amide, as the case may be, and contains diortho electron donating substitution in conjunction with meta and/or para substituents that possess a σ_p value greater than 0 and less than 1. Also described is a novel **chemiluminescent** labeling compn. comprising an ester, thioester or amide covalently and jointly bonded to (1) a carbon of a heterocyclic ring or ring system that is susceptible to attack by peroxide or mol. oxygen and (2) an aryl ring or ring system wherein the heterocyclic ring or ring system is distinguished by a heteroatom thereof in an oxidn. state which causes the attacked carbon atom to form an intermediate that decays and produces **chemiluminescence**; the aryl ring or ring system contains at least

three substituents on a six-member arom. hydrocarbon that together sterically and electronically hinder hydrolysis of the linkage, which substituents involve ortho substituent groups on the aryl in conjunction with meta and/or para substituents thereon that possess an electron withdrawing capacity characterized as a .sigma.p value greater than 0 and less than 1. Anti-TSH antibody was labeled with title compd. I.

IT 126430-78-2P 126430-80-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of **chemiluminescent** label)

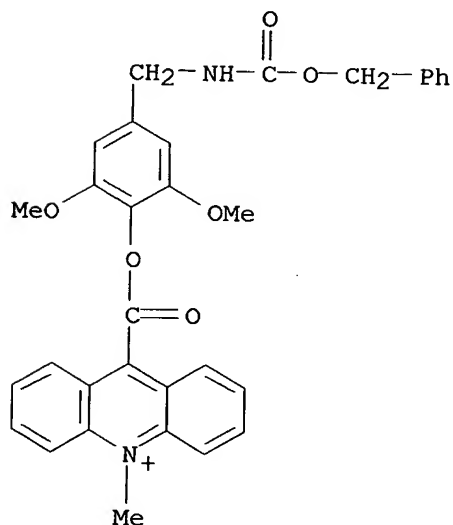
RN 126430-78-2 HCAPLUS

CN Acridinium, 9-[[2,6-dimethoxy-4-[[[(phenylmethoxy)carbonyl]amino]methyl]phenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 126430-77-1

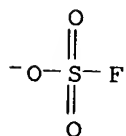
CMF C32 H29 N2 O6



CM 2

CRN 15181-47-2

CMF F O3 S



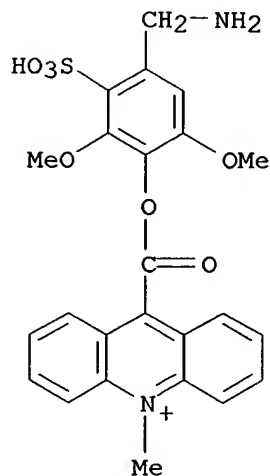
RN 126430-80-6 HCAPLUS

CN Acridinium, 9-[[4-(aminomethyl)-2,6-dimethoxy-3-sulfoxy]carbonyl]-10-

CM 1

CRN 126430-79-3

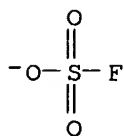
CMF C24 H23 N2 O7 S



CM 2

CRN 15181-47-2

CMF F O3 S



IT 157392-99-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as **chemiluminescent** label)

RN 157392-99-9 HCAPLUS

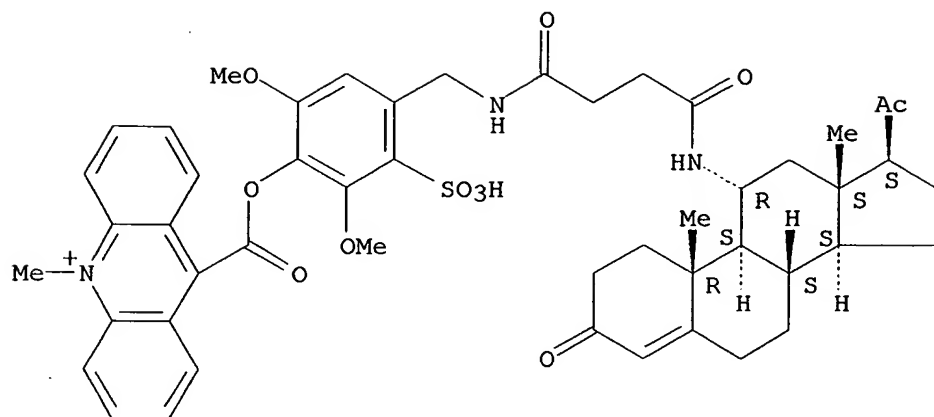
CN Acridinium, 9-[[[2,6-dimethoxy-4-[[[4-[[[11.alpha.)-3,20-dioxopregn-4-en-11-yl]amino]-1,4-dioxobutyl]amino]methyl]-3-sulphophenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157392-98-8

CMF C49 H56 N3 O11 S

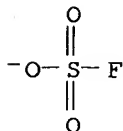
Absolute stereochemistry.



CM 2

CRN 15181-47-2

CMF F O3 S



L10 ANSWER 21 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1994:557433 HCAPLUS
 DOCUMENT NUMBER: 121:157433
 TITLE: Preparation of biotinylated **chemiluminescent** labels
 INVENTOR(S): Remakrishnan, Kastooriranganath
 PATENT ASSIGNEE(S): Nichols Institute Diagnostics, USA
 SOURCE: PCT Int. Appl., 41 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 9404538 | A1 | 19940303 | WO 1993-US7896 | 19930819 |
| W: AU, CA, FI, JP, NO, NZ | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 5395938 | A | 19950307 | US 1992-933478 | 19920821 |
| EP 656005 | A1 | 19950607 | EP 1994-908153 | 19930819 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE | | | | |
| JP 08504751 | T2 | 19960521 | JP 1993-506574 | 19930819 |
| AU 677017 | B2 | 19970410 | AU 1993-50864 | 19930819 |
| AU 9350864 | A1 | 19940315 | | |

| | | | | |
|------------------------|---|-------------------|----------------|------------|
| NO 9500632 | A | 19950407 | NO 1995-632 | 19950220 |
| FI 9500764 | A | 19950420 | FI 1995-764 | 19950220 |
| PRIORITY APPLN. INFO.: | | | US 1992-933478 | A 19920821 |
| | | | WO 1993-US7896 | W 19930819 |
| OTHER SOURCE(S): | | MARPAT 121:157433 | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds comprise a biotinyl group and a heterocyclic compd. linked via a spacer. The **chemiluminescent** labels of the invention have the ability to bind to streptavidin and/or avidin per se or to streptavidin and/or avidin conjugated with an analyte. Thus, biocytin was condensed with 2,6-dimethyl-3-chlorosulfonylphenyl 10-methylacridinium-9-carboxylate fluorosulfonate to give title compd. I. Data for use of I for quantifying progesterone using a streptavidin progesterone conjugate are given.

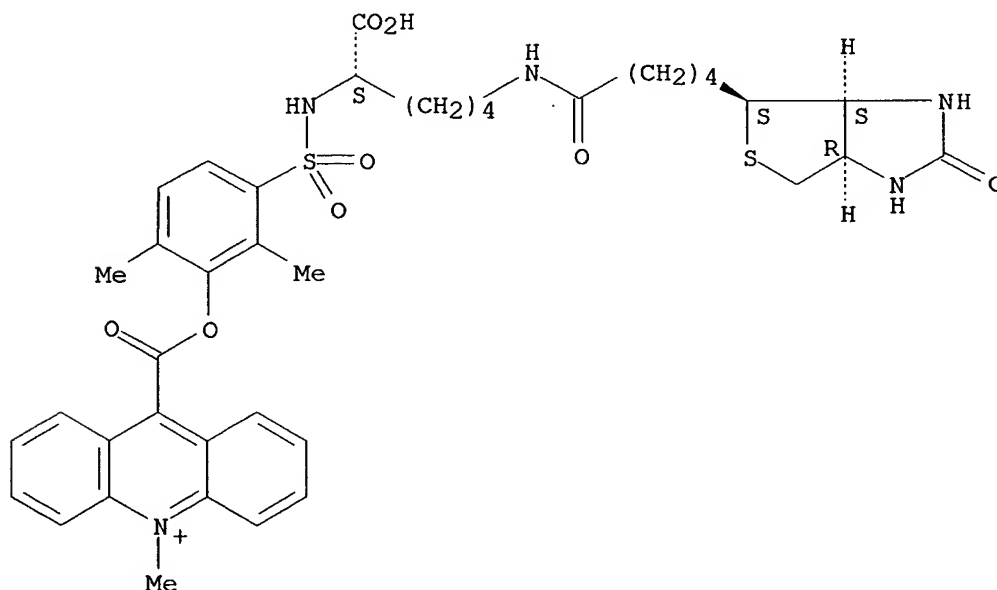
IT 157299-13-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as **chemiluminescent** label for immunoassay)

RN 157299-13-3 HCAPLUS

CN Acridinium, 9-[[[3-[[[1-carboxy-5-[[5-(hexahydro-2-oxo-1H-thieno[3,4-
 d]imidazol-4-yl)-1-oxopentyl]amino]pentyl]amino]sulfonyl]-2,6-
 dimethylphenoxy]carbonyl]-10-methyl-, [3aS-[3a.alpha.,4.beta.(R*),6a.alpha.
 .]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 22 OF 31 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:318832 HCAPLUS

DOCUMENT NUMBER: 120:318832
 TITLE: Sulfonyl-substituted **chemiluminescent** labels and their conjugates, and assays using them
 INVENTOR(S): Ramakrishnan, Kastooriranganath
 PATENT ASSIGNEE(S): London Diagnostics, Inc., USA
 SOURCE: U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 140,040, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 7
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| US 5284952 | A | 19940208 | US 1992-859995 | 19920330 |
| FR 2625565 | A1 | 19890707 | FR 1988-17502 | 19881230 |
| AU 8929270 | A1 | 19890801 | AU 1989-29270 | 19881230 |
| AU 635890 | B2 | 19930408 | | |
| DE 3891212 | T | 19910110 | DE 1988-3891212 | 19881230 |
| JP 03501772 | T2 | 19910418 | JP 1989-501385 | 19881230 |
| JP 3172522 | B2 | 20010604 | | |
| ZA 8900019 | A | 19891129 | ZA 1989-19 | 19890103 |
| GB 2232995 | A1 | 19910102 | GB 1990-14479 | 19900628 |
| GB 2232995 | B2 | 19921014 | | |
| GB 2251942 | A1 | 19920722 | GB 1992-3180 | 19920214 |
| GB 2252161 | A1 | 19920729 | GB 1992-3179 | 19920214 |
| GB 2252162 | A1 | 19920729 | GB 1992-3181 | 19920214 |
| US 5321136 | A | 19940614 | US 1992-860410 | 19920330 |

PRIORITY APPLN. INFO.:

| | | |
|----------------|----|----------|
| US 1987-140040 | B2 | 19871231 |
| US 1988-291843 | B2 | 19881229 |
| US 1989-418956 | B2 | 19891010 |
| WO 1988-US4719 | A | 19881230 |
| GB 1990-14479 | A3 | 19901230 |

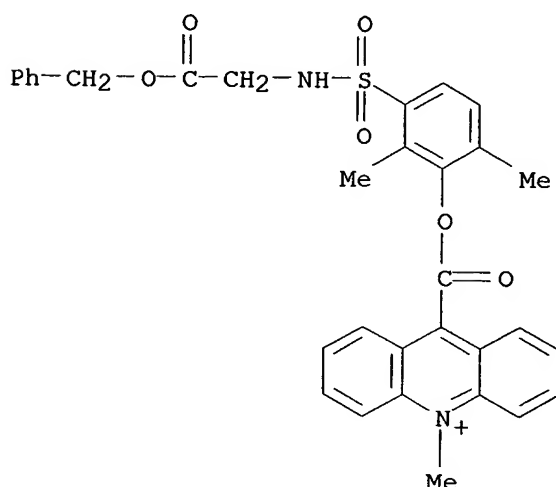
OTHER SOURCE(S): MARPAT 120:318832

AB A **chemiluminescent** labeling compn. comprises an ester, thioester or amide covalently and jointly bonded to (1) a carbon of a heterocyclic ring or ring system that is susceptible to attack by peroxide or mol. oxygen and (2) an aryl ring or ring system wherein the heterocyclic ring or ring system is distinguished by a heteroatom thereof in an oxidn. state which causes the attacked carbon atom to form an intermediate that decays and produces **chemiluminescence**. The aryl ring or ring system contains .gtoreq.3 substituents on a six-membered arom. hydrocarbon that together sterically and electronically hinder hydrolysis of the linkage, which substituents involve ortho substituent groups on the aryl in conjunction with meta and/or para -SO₂- substituents thereon. Also disclosed are the **chemiluminescent** labeling compn. conjugated with a sp. binding material, a **chemiluminescent** assay using the conjugate, and a **chemiluminescent** assay kit contg. the conjugate. Prepn. of **chemiluminescent** labels, e.g. (2,6-dimethoxy-3-chlorosulfonyl)phenyl-N-methylacridinium-9-carboxylate fluorosulfonate, is included, as is a procedure for coupling of the labels of the invention to IgG.

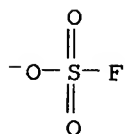
IT 155301-78-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reaction of, in **chemiluminescent** label prepn.)

RN 155301-78-3 HCAPLUS
 CN Acridinium, 9-[[2,6-dimethyl-3-[[[2-oxo-2-(phenylmethoxy)ethyl]amino]sulfonyl]phenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)
 CM 1
 CRN 155301-77-2
 CMF C32 H29 N2 O6 S



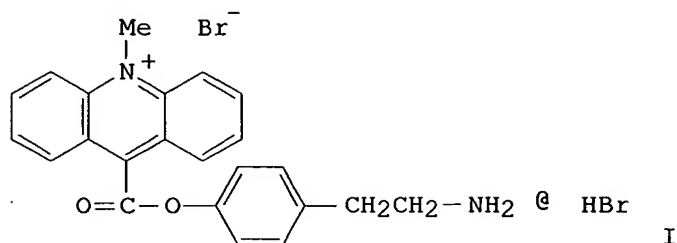
CM 2
 CRN 15181-47-2
 CMF F O3 S



L10 ANSWER 23 OF 31 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1993:115944 HCAPLUS
 DOCUMENT NUMBER: 118:115944
 TITLE: Synthesis of a new **chemiluminescent**
 immunoassay reagent - 4-(2-aminoethyl)phenyl-10-
 methylacridinium-9-carboxylate bromide (AEP-MAC)
 AUTHOR(S): Luo, Shineng; Xi, Yuefen; Jin, Jian; Xie, Minhao;
 Wang, Bocheng; Zhang, Manda; Zhang, Zhibin
 CORPORATE SOURCE: Jiangsu Inst. Nucl. Med., Wuxi, 214063, Peop. Rep.
 China
 SOURCE: Huaxue Shiji (1992), 14(5), 274-6
 CODEN: HUSHDR; ISSN: 0258-3283
 DOCUMENT TYPE: Journal

LANGUAGE:
GI

Chinese



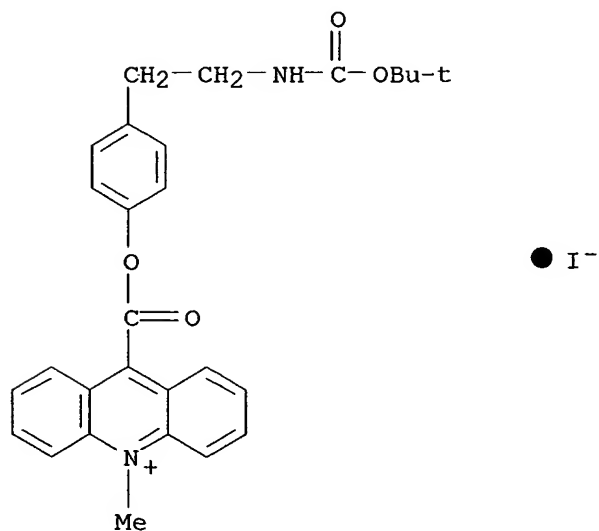
AB In this paper describes the synthesis of a new **chemiluminescent** immunoassay reagent-4-(2-aminoethyl)phenyl-10-methylacridinium-9-carboxylate bromide (I), which with an amino group can be used in the **chemiluminescent** immunoassay of materials with a carboxyl or active ester group. The elementary anal. results, the IR and mass spectra are consistent with the structure.

IT 145998-27-2

RL: RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent) (hydrolysis of)

RN 145998-27-2 HCAPLUS

CN Acridinium, 9-[[4-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]phenoxy]carbonyl]-10-methyl-, iodide (9CI) (CA INDEX NAME)



L10 ANSWER 24 OF 31 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:194326 HCAPLUS
DOCUMENT NUMBER: 116:194326

. TITLE: Preparation of 1,2,3-triazoline-3,5-dione and
 1,2,3-triazolidine-3,5-dione derivatives as
 phosphorescent or **chemiluminescent**
 dienophile reagents for analysts of vitamin D and
 analogs
 INVENTOR(S): Yamada, Sachiko; Shimizu, Masato
 PATENT ASSIGNEE(S): Biosensor Laboratories Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|-------------------|-----------------|----------|
| JP 04005287 | A2 | 19920109 | JP 1990-105046 | 19900420 |
| JP 2638253 | B2 | 19970806 | | |
| PRIORITY APPLN. INFO.: | | | JP 1990-105046 | 19900420 |
| OTHER SOURCE(S): | | MARPAT 116:194326 | | |

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I or II; X = phosphorescent chromogenic group or
 potential **chemiluminescent** group, e.g., Q, Q1, Q2; Y = spacer,
 e.g. (CH2)1, COA (CH2)m(p-C6H4)n, (CH2)1B(CH2)1; A = O, NH; B = NH, CO2,
 SO2NH, p-phenylene, etc.; l = 1-5; m = 0-5; n = 0.1], useful as dienophile
 reagents for quant. anal. or detection of cis-diene compds., particularly
 vitamin D and A and their metabolites, are prepd. Thus, a DMf soln. of
 0.6 mmol II (YX = C6H4CH2OH-p (prepn. given) was added to a benzene soln.
 of 0.4 mmol QCOCl (prepn. given) under reflux and refluxing was continued
 for 0.5 h to give 56.8% II (YX = C6H4CH2O2CQ) (III). To a cold
 (-75.degree.) suspension of 0.024 mmol vitamin D3 and 0.028 III in DMF-THF
 (1:1) and 0.5 .mu.L glacial AcOH was added 0.043 mmol Pb(OAc) with
 stirring and stirring was continued at -75.degree. for 1 h to give an
 Diels-Alder adduct (IV). Addnl. 5 I or II and 11 other adducts of vitamin
 D analogs, retinoic acid, and retinol with III or II (YX = CH2CH2Q) were
 prepd.

IT 140707-10-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as dienophile reagent for anal. of vitamin A, D, and
 analogs)

RN 140707-10-4 HCAPLUS

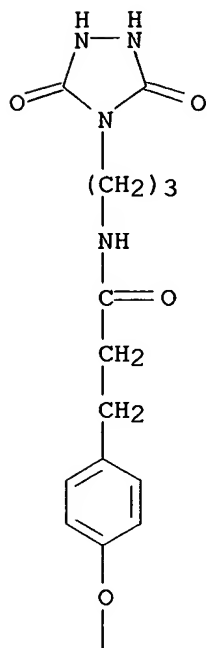
CN Acridinium, 9-[[4-[3-[[3-(3,5-dioxo-1,2,4-triazolidin-4-yl)propyl]amino]-3-
 oxopropyl]phenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX
 NAME)

CM 1

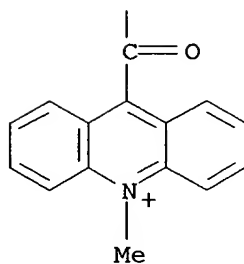
CRN 140707-09-1

CMF C29 H28 N5 O5

PAGE 1-A



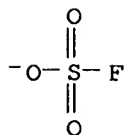
PAGE 2-A



CM 2

CRN 15181-47-2

CMF F O3 S



ACCESSION NUMBER: 1991:651479 HCAPLUS
DOCUMENT NUMBER: 115:251479
TITLE: Direct **chemiluminescence** immunoassay (CLIA)
for muramyl tripeptide phosphatidyl-ethanolamine in
plasma
AUTHOR(S): Gay, B.; Towbin, H.; Schnell, C.; Einsle, K.; Graf,
P.; Gygax, D.
CORPORATE SOURCE: Pharma. Res. Dev., Ciba-Geigy A.-G., Basel, Switz.
SOURCE: Journal of Bioluminescence and Chemiluminescence
(1991), 6(2), 73-80
CODEN: JBCHE7; ISSN: 0884-3996
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A competitive **chemiluminescent** immunoassay for quantitation of
muramyl tripeptide phosphatidyl-ethanolamine (I) in plasma has been
developed. The assay is based on the use of an acridinium ester-labeled
analog of muramyl tripeptide and a rabbit antiserum. It includes an
overnight incubation and a sepn. with a second antibody covalently coupled
to paramagnetic particles. The sensitivity of detection is 0.012 nmol/L,
the assay working range is 0.1-5 nmol/L, and the interassay coeffs. of
variation are .ltoreq.10%. Using up to 6000-fold sample dilns., a wide
working range (0.1-30,000 nmol/L) is obtained. Rat plasma samples were
collected during and one day after i.v. infusion of I. Following
infusion, the concns. in plasma declined multiphasically. Half life was
0.37 h .+- . 0.03 (alpha phase) and 1.76 .+- . 0.08 (beta phase), clearance
and vol. of distribution were 0.09 .+- . 0.02 L/h .times. kg and 0.06 .+- .
0.01 L/kg, resp. The use of an acridinium ester as a
chemiluminescent label overcomes the problems assocd. with
reagents of limited shelf life.

IT 137236-11-4P

RL: PREP (Preparation)

(prepn. of, for **chemiluminescence** immunoassay for muramyl
tripeptide phosphatidyl-ethanolamine in plasma)

RN 137236-11-4 HCAPLUS

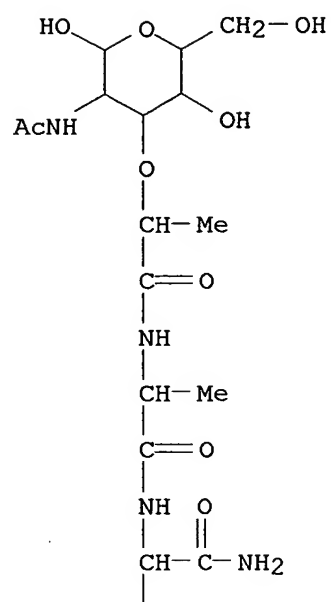
CN L-Lysine, N2-[N2-[N-(N-acetyl-.beta.-muramoyl)-L-alanyl]-D-.alpha.-
glutaminy]-N6-[3,5-dimethyl-4-[[[(10-methylacridinium-9-
yl)carbonyl]oxy]benzoyl]-, methyl sulfat (salt) (9CI) (CA INDEX NAME)

CM 1

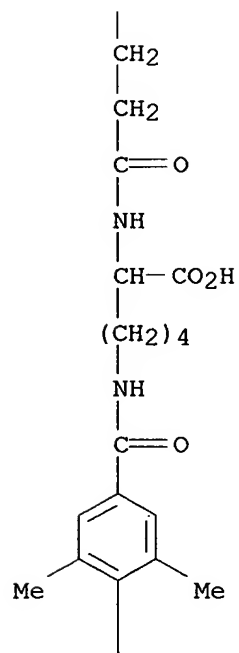
CRN 137236-10-3

CMF C49 H62 N7 O15

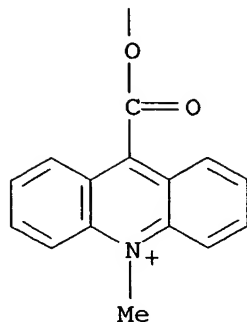
PAGE 1-A



PAGE 2-A



PAGE 3-A



CM 2

CRN 21228-90-0
CMF C H3 O4 S

Me-O-SO₃⁻

L10 ANSWER: 26 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:528989 HCAPLUS

DOCUMENT NUMBER: 113:128989

TITLE: Acridinium esters, liposomes containing them and their use in luminescence assay

INVENTOR(S): Law, Say Jong; Piran, Uri

PATENT ASSIGNEE(S): Ciba Corning Diagnostics Corp., USA

SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------------|------|----------|-----------------|----------|
| EP 353971 | A2 | 19900207 | EP 1989-307752 | 19890731 |
| EP 353971 | A3 | 19901010 | | |
| EP 353971 | B1 | 19960207 | | |
| R: BE, DE, FR, GB, IT, LU, NL | | | | |
| AU 8939033 | A1 | 19900208 | AU 1989-39033 | 19890727 |
| AU 634716 | B2 | 19930304 | | |
| JP 02096567 | A2 | 19900409 | JP 1989-199178 | 19890731 |
| JP 09025422 | A2 | 19970128 | JP 1996-179488 | 19890731 |
| CA 1339490 | A1 | 19971007 | CA 1989-607098 | 19890731 |
| AU 9332034 | A1 | 19930401 | AU 1993-32034 | 19930127 |
| AU 654754 | B2 | 19941117 | | |
| US 5656500 | A | 19970812 | US 1995-440427 | 19950512 |

PRIORITY APPLN. INFO.:

US 1988-226639 A 19880801
JP 1989-199178 A3 19890731

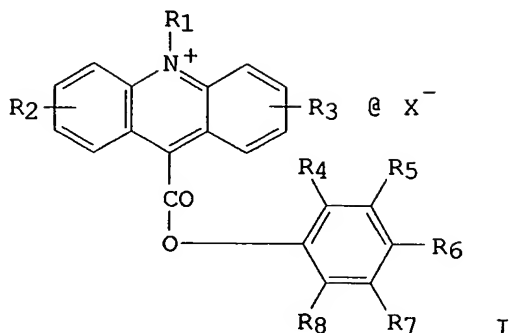
US 1992-826186 A3 19920122

US 1993-32321 A3 19930317

US 1994-325845 A1 19941019

OTHER SOURCE(S): MARPAT 113:128989

GI



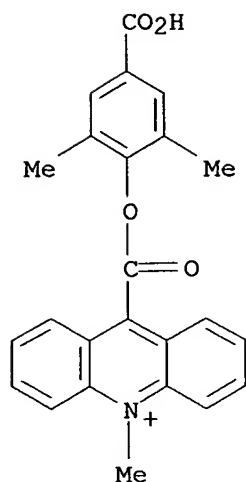
AB Hydrophilic acridinium esters I [R, R1 = alkyl, alkenyl, alkynyl, aryl, or aralkyl, which may contain .gtoreq. 1 hetero atom; R2, R3, R5, R7 = H, NH2, CO2H, etc.; R4, R8 = H, alkyl, alkenyl, alkynyl, aryl, alkoxy; R6 = CO2H, RIn, QRIn (Q = O, S, NHCSNH, etc.; I = ionizable group; X = anion; n .gtoreq. 1)] are prepd. and encapsulated in liposomes for use as **chemiluminescent** markers. The marker-contg. lumisome, uni- or multilamellar, is sensitized with antigen, hapten, antibody, nucleic acid, avidin, or other receptor. A competitive- or sandwich-type immunoassay is adapted for analytic measurement by monitoring the luminescent marker after its release from liposomes. Thus, hydrophilic 2',6'-dimethyl-4'-(sulfomethylcarbamoyl)phenyl 10-methylacridinium-9-carboxylate bromide (DMAE-AMS) was prepd. from 2',6'-dimethyl-4'-carboxyphenyl 10-methylacridinium-9-carboxylate bromide by reacting with aminoethanesulfonic acid. The DMAE-AMS was encapsulated in dipalmitoylphosphatidylethanolamine succinylthyroxine lumisomes. Monoclonal anti-T4 antibody was also prepd. and immobilized on paramagnetic particles to facilitate sepn. A competitive binding assay for T4 was performed by using a series of stds. with known increasing amts. of T4. The particles were sepd. from the supernatant magnetically by decanting, followed by washing. The luminometric measurement of DMAE-AMS was triggered by lysis of the particle-bound liposomes with 0.25 N NaOH contg. Arquad surfactant; the luminescence had a reciprocal relation with the amt. of T4 in the sample.

IT 123655-39-0

RL: ANST (Analytical study)
(liposomes contg., for luminescence anal.)

RN 123655-39-0 HCAPLUS

CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-,
bromide (9CI) (CA INDEX NAME)

● Br⁻

IT 123699-73-0P 128816-32-0P 128816-33-1P

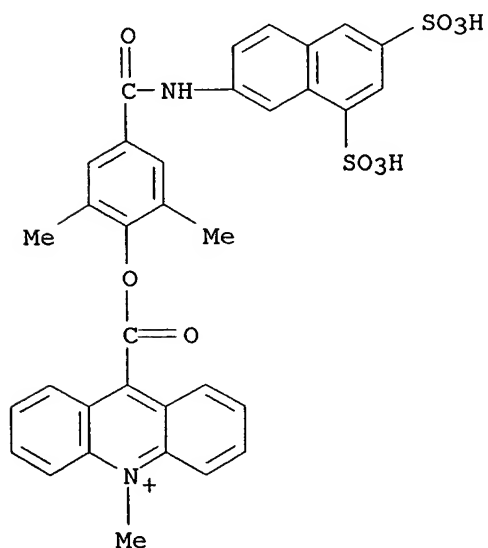
128816-34-2P 128816-35-3P 128816-36-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of and liposomes contg., for luminescence anal.)

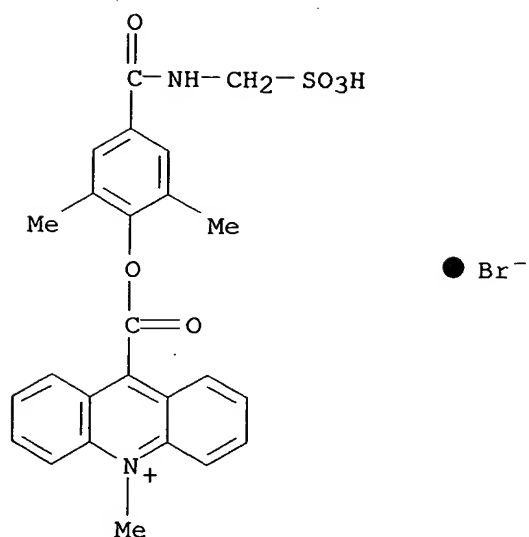
RN 123699-73-0 HCAPLUS

CN Acridinium, 9-[[4-[[[(6,8-disulfo-2-naphthalenyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

● Br⁻

RN 128816-32-0 HCAPLUS

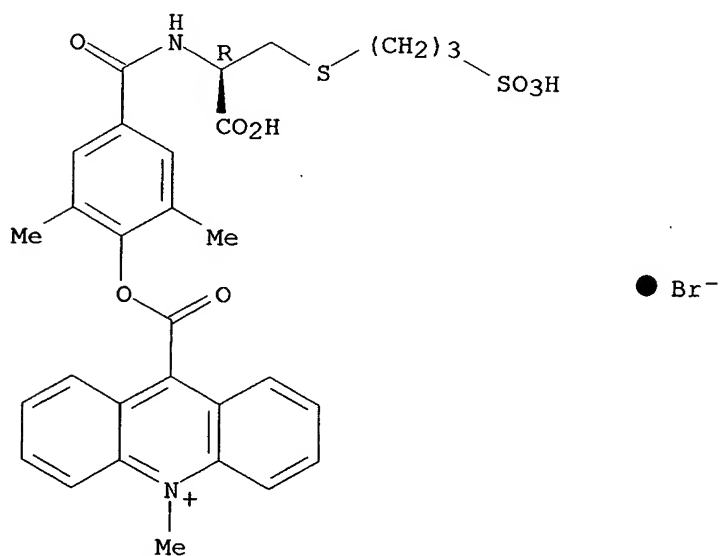
CN Acridinium, 9-[[2,6-dimethyl-4-[[[(sulfomethyl)amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



RN 128816-33-1 HCAPLUS

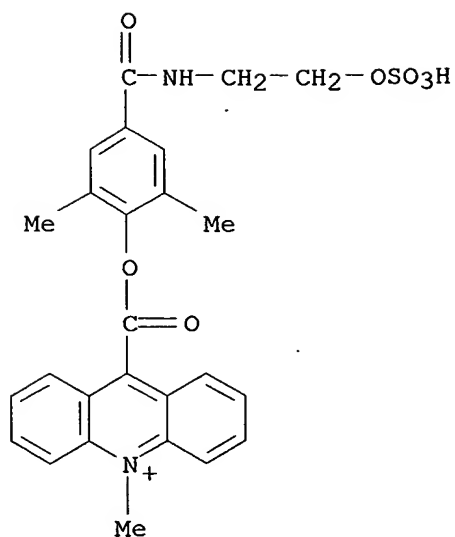
CN L-Cysteine, N-[3,5-dimethyl-4-[[(10-methylacridinium-9-yl)carbonyl]oxy]benzoyl]-S-(3-sulfopropyl)-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



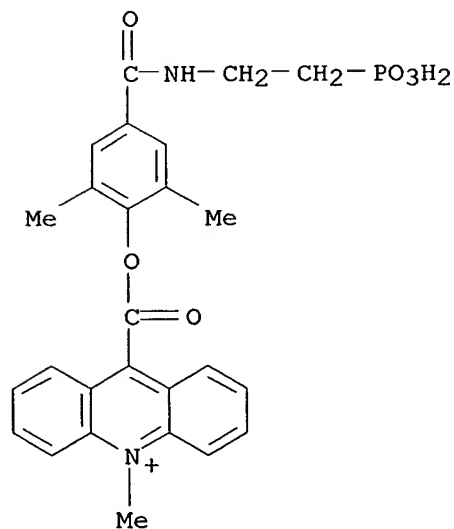
RN 128816-34-2 HCAPLUS

CN Acridinium, 9-[[2,6-dimethyl-4-[[[2-(sulfooxy)ethyl]amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

● Br⁻

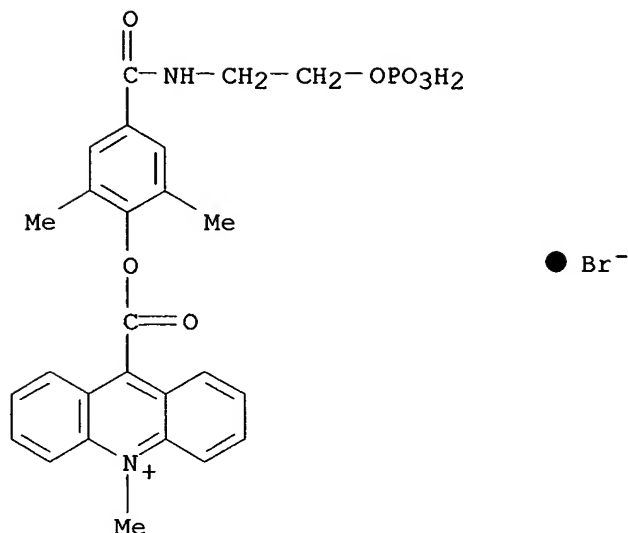
RN 128816-35-3 HCAPLUS

CN Acridinium, 9-[[2,6-dimethyl-4-[[2-(phosphonoethyl)amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)

● Br⁻

RN 128816-36-4 HCAPLUS

CN Acridinium, 9-[[2,6-dimethyl-4-[[2-(phosphonoethyl)amino]carbonyl]phenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



L10 ANSWER 27 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:213573 HCAPLUS

DOCUMENT NUMBER: 112:213573

TITLE: Improved **chemiluminescent** esters, thioesters, and amides, their preparation, and assays using them

INVENTOR(S): McCapra, Frank; Beheshti, Iraj; Hart, Russell C.; Koelling, Harlen; Patel, Ashokkumar; Ramakrishnan, Kastooriranganath

PATENT ASSIGNEE(S): London Diagnostics, Inc., USA

SOURCE: Eur. Pat. Appl., 85 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 7

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 322926 | A2 | 19890705 | EP 1988-121915 | 19881230 |
| EP 322926 | A3 | 19910320 | | |
| EP 322926 | B1 | 19990811 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| FR 2625565 | A1 | 19890707 | FR 1988-17502 | 19881230 |
| WO 8906231 | A1 | 19890713 | WO 1988-US4719 | 19881230 |
| W: AT, AU, BG, BR, CH, DE, DK, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, NL, NO, RO, SE, SU | | | | |
| RW: BJ, CF, CG, CM, GA, ML, MR, SN, TD, TG | | | | |
| AU 8929270 | A1 | 19890801 | AU 1989-29270 | 19881230 |
| AU 635890 | B2 | 19930408 | | |
| DE 3891212 | T | 19910110 | DE 1988-3891212 | 19881230 |
| JP 03501772 | T2 | 19910418 | JP 1989-501385 | 19881230 |
| JP 3172522 | B2 | 20010604 | | |
| IL 88848 | A1 | 19940227 | IL 1988-88848 | 19881230 |
| EP 916658 | A1 | 19990519 | EP 1998-123411 | 19881230 |

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

| | | | | |
|------------|----|----------|----------------|----------|
| AT 183311 | E | 19990815 | AT 1988-121915 | 19881230 |
| ES 2134185 | T3 | 19991001 | ES 1988-121915 | 19881230 |
| ZA 8900019 | A | 19891129 | ZA 1989-19 | 19890103 |
| GB 2232995 | A1 | 19910102 | GB 1990-14479 | 19900628 |
| GB 2232995 | B2 | 19921014 | | |
| GB 2251942 | A1 | 19920722 | GB 1992-3180 | 19920214 |
| GB 2252161 | A1 | 19920729 | GB 1992-3179 | 19920214 |
| GB 2252162 | A1 | 19920729 | GB 1992-3181 | 19920214 |

PRIORITY APPLN. INFO.:

| | | |
|----------------|----|----------|
| US 1987-140040 | A | 19871231 |
| US 1988-291843 | A | 19881229 |
| EP 1988-121915 | A3 | 19881230 |
| WO 1988-US4719 | A | 19881230 |
| GB 1990-14479 | A3 | 19901230 |

AB Specific binding assays are disclosed which utilize a **chemiluminescent** compd. which has increased stability in aq. soln. The **chemiluminescent** moiety is an ester, thioester or amide in which the ester, thioester or amide linkage is between (1) a heterocyclic ring or ring system contg. a C atom to which the linkage is attached, wherein the heteroatom within the heterocyclic ring or ring system is in an oxidn. state which renders such C atom susceptible to attack by peroxide or O₂ to form an intermediate which decays to produce **chemiluminescence**, and (2) an aryl ring or ring system. The aryl ring or ring system contains .gtoreq.1 substituted 6-member ring. The substituted 6-member ring has .gtoreq.2 substituent groups, where .gtoreq.2 of said substituent groups sterically hinder hydrolysis of said linkage. One or more of the substituent groups which sterically hinder hydrolysis of said linkage may be an electron-withdrawing group. The substituted 6-member ring may have .gtoreq.1 addnl. substituent groups in addn. to the substituent groups which sterically hinder hydrolysis of the linkage. Such addnl. substituent groups may also be an electron withdrawing group. The C atoms in the heterocyclic ring or ring system, to which the linkage is attached, may also have a secondary substituent of the formula R_nX (X is selected from the group consisting of O, N, S and C; R is any group; n is a no. such that X has proper valency). Other **chemiluminescent** moieties are disclosed which are characterized by a heterocyclic ring or ring system and a secondary substituent of the formula R_nX, with the ester, thioester or amide linkage being between the heterocyclic ring or ring system and a leaving group. The disclosed **chemiluminescent** moieties can also include substituents at peri positions within the heterocyclic ring or ring system. Compns. and kits including the **chemiluminescent** moieties are provided, as are immunoassays employing the moieties. Stability as a function of time and pH for some of the prepd. moieties and IgG conjugates are included. Thus, (2,6-dimethoxy-3-chlorosulfonyl)phenyl-N-methyl-acridan-9-ethoxy-9-carboxylate (I) was prepd. by reacting (2,6-dimethoxy-3-chlorosulfonyl)phenyl-N-methyl-acridinium-9-carboxylate with K t-butoxide in abs. EtOH. I was conjugated to affinity-purified goat anti-TSH antibody and used in an immunoassay for TSH. Addn. of HNO₃ to the assay mixt. contg. the labeled antibody caused the C9 ethoxy group to cleave from the acridinium mol. before the **chemiluminescent** reaction was triggered by NaOH. A std. curve for the assay is shown.

IT 126430-78-2P 126430-80-6P 126430-82-8P

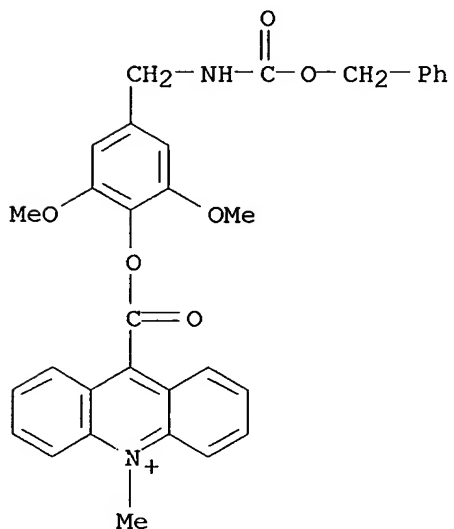
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of **chemiluminescent** label with increased resistance to hydrolysis)

RN 126430-78-2 HCAPLUS
CN Acridinium, 9-[[2,6-dimethoxy-4-[[[(phenylmethoxy)carbonyl]amino]methyl]phenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

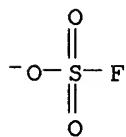
CM 1

CRN 126430-77-1
CMF C32 H29 N2 O6



CM 2

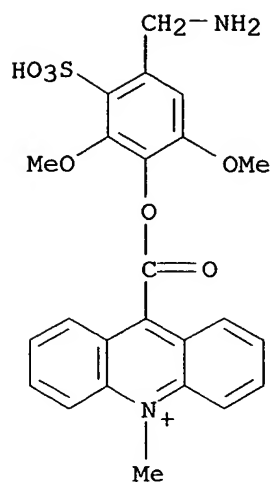
CRN 15181-47-2
CMF F O3 S



RN 126430-80-6 HCAPLUS
CN Acridinium, 9-[[4-(aminomethyl)-2,6-dimethoxy-3-sulfophenoxy]carbonyl]-10-methyl-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

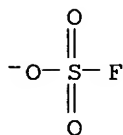
CRN 126430-79-3
CMF C24 H23 N2 O7 S



CM 2

CRN 15181-47-2

CMF F O3 S



RN 126430-82-8 HCAPLUS

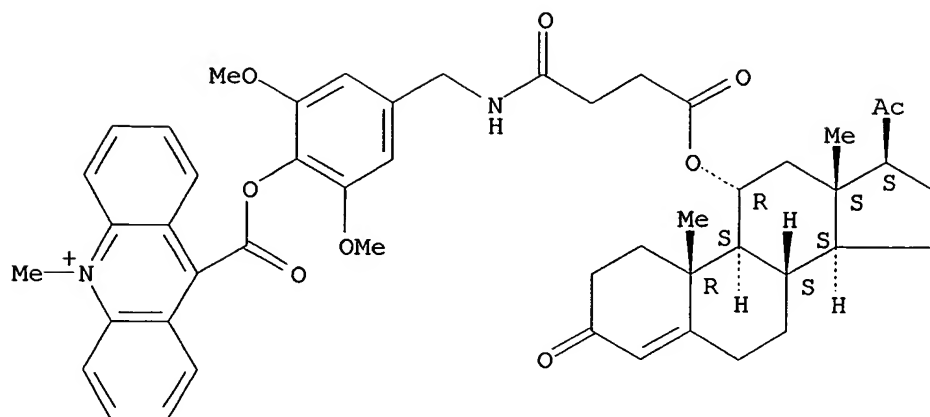
CN Pregn-4-ene-3,20-dione, 11-[4-[[[3,5-dimethoxy-4-[[[(10-methylacridinium-9-yl)carbonyl]oxy]phenyl]methyl]amino]-1,4-dioxobutoxy]-, (11.alpha.)-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 126430-81-7

CMF C49 H55 N2 O9

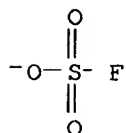
Absolute stereochemistry.



CM 2

CRN 15181-47-2

CMF F O3 S



L10 ANSWER 28 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1989:609233 HCAPLUS

DOCUMENT NUMBER: 111:209233

TITLE: Novel poly-substituted aryl acridinium esters and their use in immunoassay

AUTHOR(S): Law, Say Jong; Miller, Thomas; Piran, Uri; Klukas, Carol; Chang, Steve; Unger, John

CORPORATE SOURCE: Ciba-Corning Diagn., East Walpole, MA, 02032, USA

SOURCE: Journal of Bioluminescence and Chemiluminescence (1989), 4(1), 88-98

CODEN: JBCHE7; ISSN: 0884-3996

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Acridinium ester analogs have been developed for use as nonisotopic labels in immunoassay procedures, thereby providing an alternative to RIA. The acridinium esters can be utilized in immunoassays of the sandwich, competitive, and receptor formats, and hydrophilic acridinium esters have been encapsulated in liposomes for immunoassays. The uses of the compds. and immunoassay techniques are illustrated by assays for TRH, thyroxine, and vitamin B12.

IT 123655-38-9P 123655-39-0P 123699-73-0P

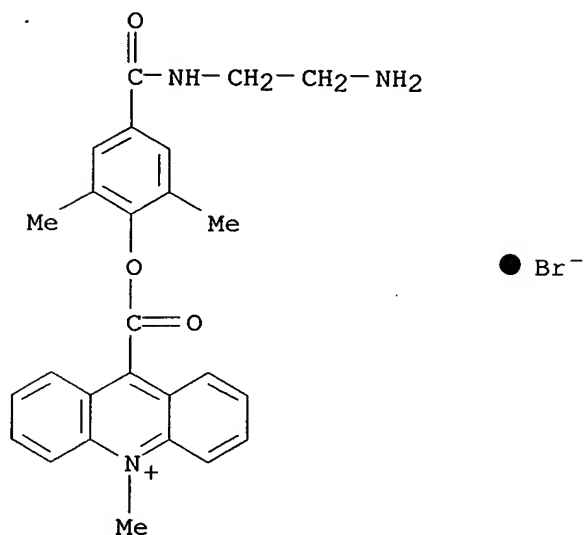
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as label for **chemiluminescent** immunoassay)

RN 123655-38-9 HCAPLUS

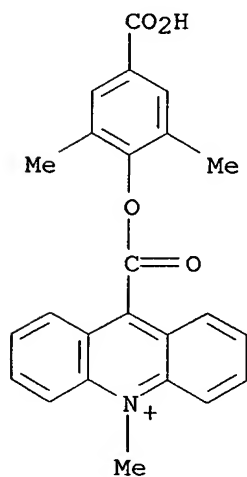
CN Acridinium, 9-[[4-[[[(2-aminoethyl)amino]carbonyl]-2,6-

dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



RN 123655-39-0 HCAPLUS

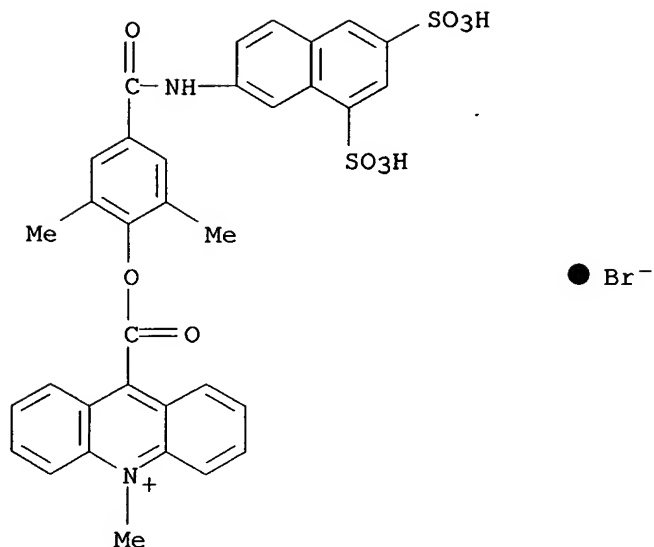
CN Acridinium, 9-[(4-carboxy-2,6-dimethylphenoxy)carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 123699-73-0 HCAPLUS

CN Acridinium, 9-[[[4-[(6,8-disulfo-2-naphthalenyl)amino]carbonyl]-2,6-dimethylphenoxy]carbonyl]-10-methyl-, bromide (9CI) (CA INDEX NAME)



L10 ANSWER 29 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1988:143565 HCAPLUS

DOCUMENT NUMBER: 108:143565

TITLE: **Chemiluminescence** immunoassay for progesterone in plasma incorporating acridinium ester labelled antigen

AUTHOR(S): Miller, S. A.; Morton, M. S.; Turkes, A.

CORPORATE SOURCE: Coll. Med., Univ. Wales, Cardiff, CF4 4XX, UK

SOURCE: Annals of Clinical Biochemistry (1988), 25(1), 27-34

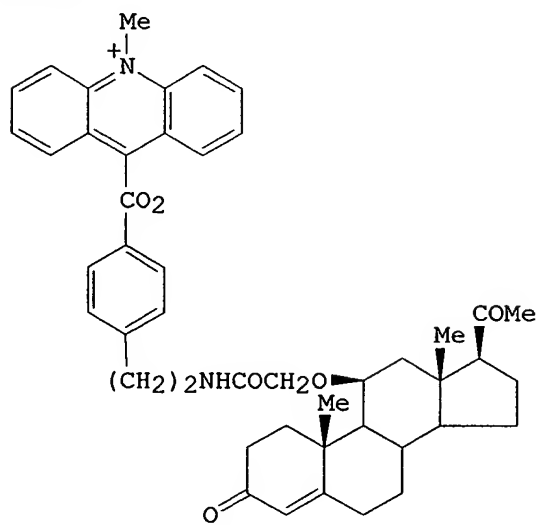
CODEN: ACBOBU; ISSN: 0004-5632

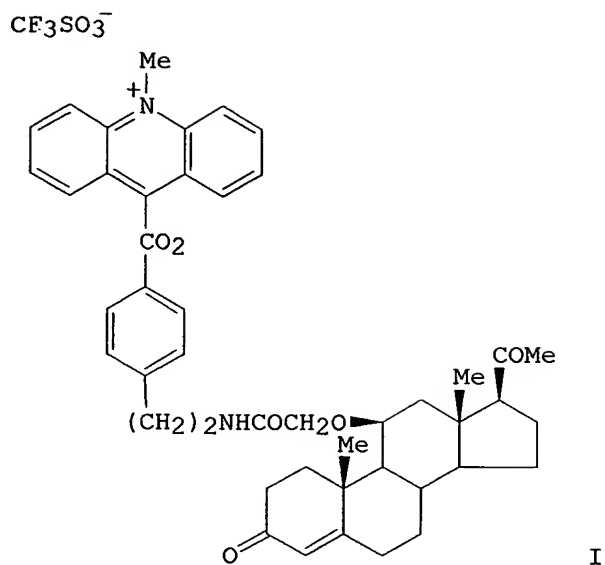
DOCUMENT TYPE: Journal

LANGUAGE: English

GI

CF₃SO₃⁻





AB A sensitive, solid-phase **chemiluminescence** immunoassay suitable for detg. progesterone concns. in plasma was developed. The solid-phase antiserum was prepd. by coupling a monoclonal progesterone-antibody, raised against a progesterone-11.alpha.-hemisuccinyl/bovine serum albumin conjugate, to CNBr-activated cellulose. I was used as the **chemiluminescent** label. The assay had a lower limit of sensitivity of 3 pg/assay tube and satisfied accepted validation criteria. Progesterone concns. detd. by **chemiluminescence** assay were in good agreement not only with a RIA in routine use but also with a gas chromatog.-mass spectrometry procedure.

IT **113578-24-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as label for **chemiluminescence** immunoassay)

RN 113578-24-8 HCAPLUS

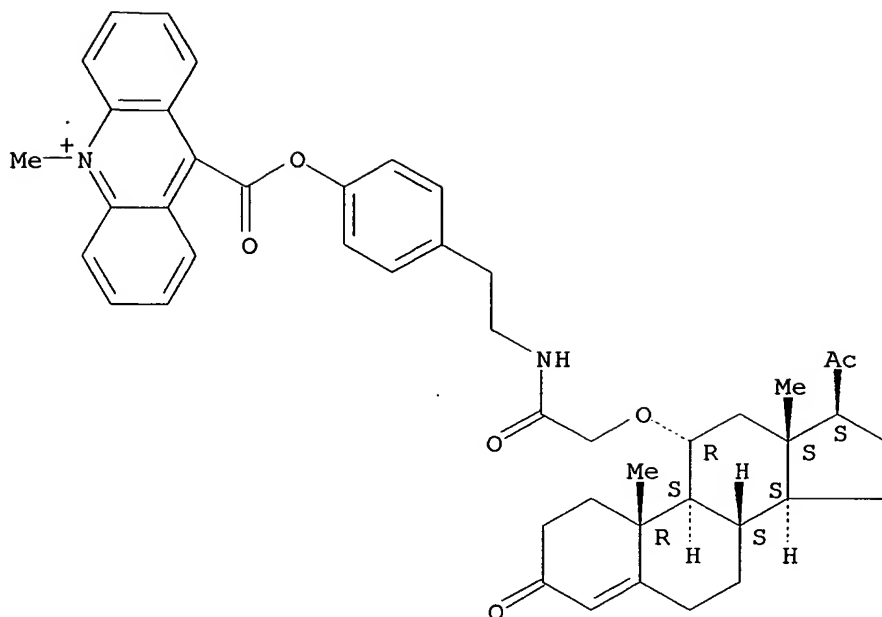
CN Acridinium, 9-[[4-[2-[[[(11.alpha.)-3,20-dioxopregn-4-en-11-yl]oxy]acetyl]amino]ethyl]phenoxy]carbonyl]-10-methyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 113578-23-7

CMF C46 H51 N2 O6

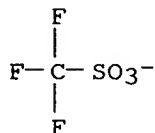
Absolute stereochemistry.



CM 2

CRN 37181-39-8

CMF C F3 O3 S



L10 ANSWER 30 OF 31 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1988:143480 HCAPLUS

DOCUMENT NUMBER: 108:143480

TITLE: **Chemiluminescent** labels for steroid immunoassaysAUTHOR(S): Klingler, Wolfgang; Wiegand, Gabriele; Knuppen, Rudolf
CORPORATE SOURCE: Inst. Biochem. Endokrinol., Med. Univ. Luebeck, Luebeck, D-2400, Fed. Rep. Ger.SOURCE: Journal of Steroid Biochemistry (1987), 27(1-3), 41-5
CODEN: JSTBBK; ISSN: 0022-4731

DOCUMENT TYPE: Journal; General Review

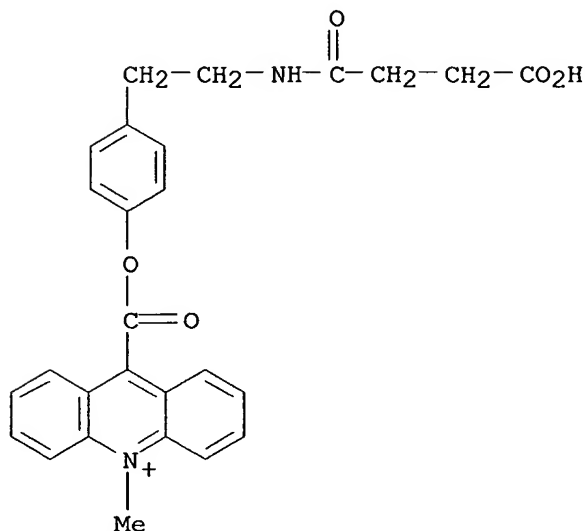
LANGUAGE: English

AB A review, with 35 refs., on the luminescence immunoassay. Three classes of substances have been found to yield reasonable results, i.e. aminophthalhydrazides, aminonaphthohydrazides, and acridinium esters. Examples of application are shown.

IT 113739-38-1

RL: BIOL (Biological study)
(as luminescent label for progesterone immunoassay)

RN 113739-38-1 HCAPIUS
CN Acridinium, 9-[[4-[2-[(3-carboxy-1-oxopropyl)amino]ethyl]phenoxy]carbonyl]-10-methyl- (9CI) (CA INDEX NAME)



L10 ANSWER 31 OF 31 HCAPIUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:606723 HCAPIUS

DOCUMENT NUMBER: 103:206723

TITLE: **Chemiluminescence** immunoassay of plasma progesterone, with progesterone-acridinium ester used as the labeled antigen

AUTHOR(S): Richardson, A. P.; Kim, J. B.; Barnard, G. J.; Collins, W. P.; McCapra, F.

CORPORATE SOURCE: Sch. Chem. Mol. Sci., Univ. Sussex, Falmer, BN1 9QJ, UK

SOURCE: Clinical Chemistry (Washington, DC, United States) (1985), 31(10), 1664-8
CODEN: CLCHAU; ISSN: 0009-9147

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This simple solid-phase **chemiluminescence** immunoassay for measurement of progesterone [57-83-0] in exts. of venous plasma has sensitivity and precision similar to that of conventional RIA with use of a tritiated antigen. The labeled antigen, 11.alpha.-progesterone-2-succinoyltyramine-4-(10-methyl)-acridinium-9-carboxylate iodide [**99160-44-8**] and a monoclonal antibody to progesterone-11.alpha.-succinyl-bovine serum albumin are incubated with a 100 .mu.L aliquot of plasma ext. (equiv. to 20 .mu.L of plasma) and 50 .mu.L of a suspension of an IgG fraction of a donkey antiserum to mouse Igs, covalently attached to cellulose particles. After the antibody-binding reaction (60 min at 4.degree.), 1 mL of phosphate buffer is added to each tube, the tubes are centrifuged (5 min, 1500 g), and the supernatant fluid is aspirated. The washing step is repeated and dild. HCl (50 mmol/L, 50 .mu.L) is added to the pellet. Luminescence is initiated by oxidn. with dil. NaOH/H₂O₂. The signal is integrated over 10 s. The light yield is inversely proportional

to the progesterone concn. in the std. or sample. The sensitivity was 0.64 mM. Intraassay and interassay relative std. deviations were 7.2-12.5 and 12.4-23.3%, resp.

IT 99160-44-8P

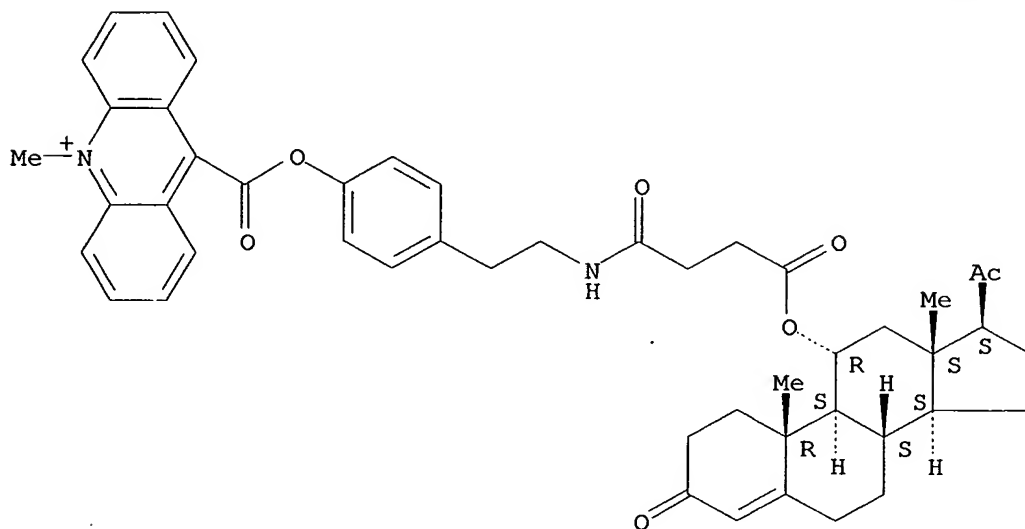
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as **chemiluminescent** marker for progesterone immunoassay)

RN 99160-44-8 HCAPLUS

CN Pregn-4-ene-3,20-dione, 11-[4-[[2-[4-[[[(10-methylacridinium-9-yl)carbonyl]oxy]phenyl]ethyl]amino]-1,4-dioxobutoxy]-, iodide, (11.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

● I⁻